25th January 2023

# PhD contract offer

## Thermoelectric properties of novel chalcogenide semiconductors with a complex crystal structure

## General information

**Workplace:** Institut Jean Lamour, Nancy, France
**Type of contract:** PhD contract
**Contract period:** 36 months
**Expected date of employment:** October 2023
**Proportion of work:** Full time
**Remuneration:** 2044 € (gross salary)
**Desired level of education:** Master's degree in solid-state physics, solid-state chemistry or material science
**Experience required:** /

## Missions / Activities

**General context**

Thermoelectric (TE) materials convert a temperature difference into an electrical current and vice versa. This solid-state energy conversion offers many advantages such as the absence of moving parts, the absence of vibration or emission of greenhouse gases. The main obstacle to a wider deployment of this technology is the low conversion efficiency of TE devices which remain lower than those obtained by other technologies. The efficiency is directly related to the transport properties of the TE materials that make up the active part of these devices. A good TE material must have, at a given temperature T (K), a high Seebeck coefficient S (or thermoelectric power, V/K), a low thermal conductivity C (W/mK) so as to maintain the temperature gradient and low electrical resistivity E (Ω.m) to minimize the Joule effect. These desirable properties are expressed through the dimensionless thermoelectric figure of merit $ZT = (S^2T)/(C.E)$. This factor is used to assess the quality of a material for TE applications. The manufacture of high-performance TE devices necessarily involves obtaining materials with ZT greater than 1.

A first possible strategy to improve the thermoelectric performances of new materials is to optimize the power factor $S^2/E$ by judiciously modifying the parameters of the electronic band structure. Among the known mechanisms, the introduction of specific impurities qualified as resonant or the convergence of several electronic bands are particularly effective mechanisms. A second strategy lies in the identification of new materials which naturally have very low values of thermal conductivity or whose values can be modulated by playing on the structural disorder, for example.

**Objectives and work program**

As part of this second strategy, this thesis subject aims to study the transport properties of new chalcogenide semiconductors (that is, based on S, Se or Te) with a complex crystalline structure which combine good electronic properties and very low thermal conductivity values. The activities of the successful candidate will focus on synthesis, physical and chemical characterizations (crystal structure, microstructure, chemical composition), measurements of transport properties (thermal, electrical, galvanomagnetic, thermodynamic and magnetic fields at low and high temperatures; 2 – 1000 K) of these compounds in polycrystalline form but also in single-crystalline form. Polycrystalline compounds

will be synthesized by powder metallurgy in sealed silica tubes or by high-energy mechanical ball milling. The single crystals will be synthesized either by a Bridgman-type growth technique or by a flux method.

The crystal structure and the chemical composition and homogeneity will be determined using the latest-generation instruments possessed by the institute's competence centers (X-ray diffraction on powder and single-crystal, Laue diffraction of CC Xγ, scanning and transmission electron microscopy and Castaing electron microprobe of CC 3M). Complementary studies of the crystal structure on large instruments (X-rays synchrotron and neutron diffraction, at ESRF and at ILL in Grenoble) will also be carried out in order to further specify the important crystallographic characteristics (characterization of the disorder or position of the dopants in the structure for example).

The transport properties will be measured over a wide range of temperatures (2 – 1000 K) using the substantial instrumentation available in the host team. While high-temperature measurements will make it possible to determine the thermoelectric performance of the compounds synthesized, low-temperature measurements will shed important light on the microscopic mechanisms that govern their electrical and thermal transport. The study of very low lattice thermal conductivities will be deepened by measurements of inelastic neutron/X-ray scattering on powder and on single crystals (ILL and ESRF in Grenoble).

## Work context

The thesis will take place mainly at the Institut Jean Lamour in Nancy, under the supervision of Christophe Candolfi (director) and Soufiane El Oualid (co-director).
At the end of the thesis, the student will have learned to master the techniques of manufacturing thermoelectric materials, to characterize their structural and chemical properties using state-of-the-art instruments and to measure their performance as a function of temperature.

## Skills

- Holder of an engineering degree or a Master 2 in the field of materials science.
- Knowledge of solid-state physics or chemistry and characterization of materials.
- Fluent English.

## About Institut Jean Lamour

The Institute Jean Lamour (IJL) is a joint research unit of CNRS and Université de Lorraine.
Focused on materials and processes science and engineering, it covers: materials, metallurgy, plasmas, surfaces, nanomaterials and electronics.
It regroups 183 researchers/lecturers, 91 engineers/technicians/administrative staff, 150 doctoral students and 25 post-doctoral fellows.
Partnerships exist with 150 companies and our research groups collaborate with more than 30 countries throughout the world.
Its exceptional instrumental platforms are spread over 4 sites; the main one is located on Artem campus in Nancy.

## Constraints and risks

The position you are applying for is located in a sector relating to the protection of scientific and technical potential. It therefore requires, in accordance with the regulations, that your arrival be authorized by the competent authority of the Ministry of Higher Education, Research and Innovation.
Risks of exposure to electromagnetic and ionizing radiations, risks associated with high temperatures.

## Application

Applicants are invited to send a CV, a cover letter together with diploma copies and grades to:
Dr. Christophe Candolfi, christophe.candolfi@univ-lorraine.fr
Dr. Soufiane El Oualid, soufiane.el-oualid@univ-lorraine.fr