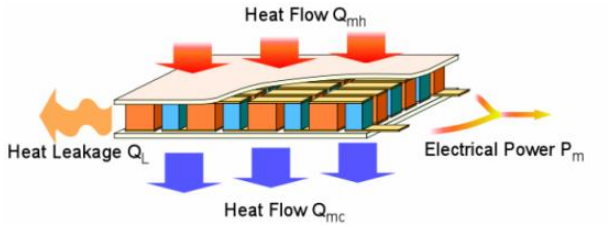


# Post Doctoral Position ICG Montpellier : Low Cost Thermoelectric Heusler Alloys

**A Post-doctoral position of one year is available in the Theoretical and Physical Chemistry Department of the Charles Gerhardt Institute in Montpellier (ICGM), France under the supervision of Pr. Philippe Jund.**

Thermoelectric cooling (TEC) based on materials with a dimensionless thermoelectric figure of merit ($Z=S^2\sigma/\kappa$) larger than 0.2 at 300 K can compete with absorption refrigeration while TEC based on materials with ZT larger than 1 at 300 K can compete with current air conditioning systems. Such materials can also be the basis of small-scale thermoelectric generators (TEG) to power the wireless sensors required by applications like the “Internet of Things” or the “Factory 4.0”.

The **Heusler alloy $Fe_2VAl$** could be considered as a substitute to $Bi_2Te_3$ (the most used but toxic material) for TEC & TEG applications at 300K. Its chemical elements are indeed non-toxic and inexpensive. Moreover, $Fe_2VAl$ can be obtained both as *n*-type and *p*-type and the combination of its Seebeck coefficient and electrical conductivity is better than in $Bi_2Te_3$. However, its thermal conductivity $\kappa$ (28 W $m^{-1}$ $K^{-1}$ at 300 K in pristine $Fe_2VAl$) is unfavorable to applications since it is an order of magnitude larger than in $Bi_2Te_3$.

To solve this problem, the research consortium constituted by the Institut de Chimie et de Matériaux Paris-Est (ICMPE, Thiais) and the Institut Charles Gerhardt Montpellier (ICGM) proposes to reduce the thermal conductivity in $Fe_2Val$ within the frame of **the ANR project LoCoThermH (2018-2022).**

To intensify scattering of the phonons at an atomic scale, solid solutions with multiple substitutions like $Fe_{2-x}M_xV_{1-y}T_yAl_{1-z}X_z$ (M, T, X = other elements of the periodic table) will be experimentally examined. The choice of these substituent(s) will be guided by first principles calculations of the thermoelectric properties, which will be carried out in the frame of the Density Functional Theory (DFT).

This **DFT screening** (using the code **VASP** and the **BoltzTrap** program) constitutes the principal work of the successful applicant who should have a solid background in solid state chemistry/physics as well as in computational material science.

The position is available immediately until a suitable candidate is identified. Applicants should send their CV and application letters, including name and addresses of contact persons for recommendation to Pr. Philippe Jund: **philippe.jund@umontpellier.fr**