



Master 2 Internship proposal

Main Institution: ICGM - University of Montpellier Associated partner: Hutchinson company 	 Institut Charles Gerhardt Montpellier
Supervisor:	<i>Name: Jund First name: Philippe</i> <i>Email: philippe.jund@umontpellier.fr</i> <i>Position: Professor of Theoretical Chemistry</i>

TITLE: Thermoelectric functionalization of silica based superinsulating materials via *ab initio* simulations

Keywords: first principles calculations, electronic properties, thermoelectrics, thermal insulating materials

Description:
Hutchinson is interested in functionalizing its proprietary superinsulating materials to keep up with evolving demand. The combination of various functions inside an all-in-one product is long awaited by the customers of the transport. In that direction the integration of thermoelectric materials inside the thermal insulating structure would enable the production of electricity without adding extra and inconvenient volume. Nevertheless most of the thermal insulating materials are also electrical insulators, thus the aim of this internship is twofold:
- conclude the relaxation of the pure silica based material started during a previous Master 2 Internship in 2020
- determine *in silico* the most promising doping elements in order to obtain the best thermoelectric conversion
The work will be performed with existing DFT based computer codes (mostly but not exclusively VASP) and some specific programs permitting to determine the Seebeck coefficient and the electrical conductivity (BoltzTrap): all these programs are available at the host Institution. The trainee should thus appreciate computer simulations and should have a solid background in Materials Science.
In parallel of the computer screening, experimental tests on several compounds will be performed by the Hutchinson Company, permitting to have an exhaustive investigation of the problematic.
The work exposed in this proposal will be supervised by Pr. Philippe Jund at the Institut Charles Gerhardt of Montpellier in the group of Theoretical Chemistry and Modeling and Jérémy Guazzagaloppa of the Hutchinson Company.

Related URLs: www.icgm.fr/philippe-jund

Additional info: the trainee will be located at the ICGM in Montpellier (regular video meetings with Hutchinson (Chalette/Loing) will be scheduled

Duration: from 01/02/2021 to 30 /07/2021
Gratification: 920 (€/month)
PhD opportunity: CIFRE PhD (in collaboration with Hutchinson)