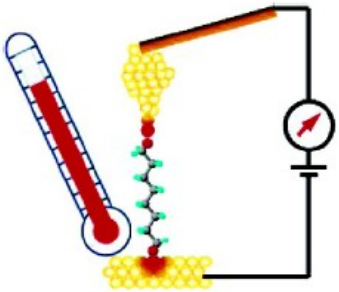
PhD offer funded by : Future and Emerging Technologies – 2016

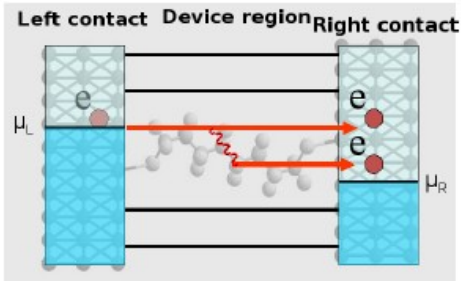
Net salary : ~ 1500 euros/months

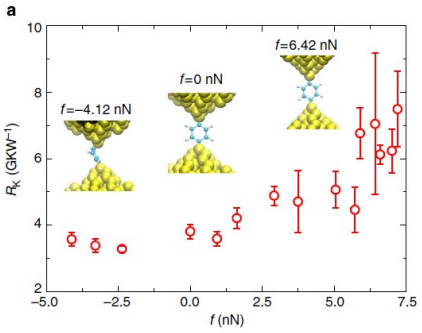
Starting date : after 1st January 2018

# Modelling electro-thermal energy transport in nano-devices for cooling applications

The phD offer is part of an European project gathering theoreticians and experimentalists all experts in nanoscale thermal and electronic transport. This project tackles innovative non-equilibrium energy management technologies for ultra sensitive infrared detectors, efficient harvesters and compact coolers for information and communication technologies (ICT). At the limits of heat management, the performance of electrothermal energy devices are limited by near field heat flux and electronic and thermal energy fluxes at the molecular length scales. A theoretical understanding of the individual non-equilibrium energy/particle channels and inter-channel couplings is essential to imagine new and efficient thermal management devices. We plan to address non-linear transport in molecular junctions starting from state-of-the-art theoretical modelling. This project combines synergies in theory, experiment and technology-development covering different fields from chemistry to physics and electronics.






The successful candidate will investigate the electro-thermal transport properties of molecular junctions, in relation with the experimentalist partners of the project, in Germany, United Kingdom and Switzerland. Interactions with researchers working at the CETHIL, INSA Lyon will also be conducted all along the project.

Electronic transport will be studied on the basis of the density functional based tight-binding method (DFTB) in conjunction with the non-equilibrium Green's function formalism. DFTB is an approximate density functional theory (DFT) method used to compute the electronic structure of complex metal-molecule-metal junctions, which allows determining the electronic conductance, the thermopower and the electronic part of the thermal conductance.

Molecular dynamics (MD), which offers the possibility to probe phonon thermal transport across the molecule, as a function of the junction length. We will also quantify the importance of non-equilibrium effects and compare the out-of-equilibrium conditions to Landauer-Büttiker estimations. Inelastic transport and non-linear response will be included on different levels, in systematic and consistent way using non-equilibrium MD.

The successfull candidate should hold a Master degree in Physics, Chemistry or Material Science. He/she should have a pronounced taste for theoretical modelling, good knowledge of basic programming and very good communication skills in English (oral and written). The successfull candidate will work at the Institute Lumière Matière in Lyon, in the team «Modélisation de la matière Condensée et Interfaces».

Interested candidates should send a resume, marks and ranking in the Master degree, a letter of motivation, at least one letter of recommendation and the names and contact of two scientific referents in a single pdf document to Thomas Niehaus (thomas.niehaus@univ-lyon1.fr) and Samy Merabia (samy.merabia@univ-lyon1.fr) . Inquiries about the post are welcome.