Proposition de stage / Internship proposal

Date de la proposition : 10/10/2021

Responsable du stage / *internship supervisor*:

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Nom du Laboratoire / *laboratory name*:

Etablissement / *institution* : C2N Code d'identification : UMR 9001

Site Internet / *web site*: https://www.c2n.universite-paris-saclay.fr/fr/

Adresse / *address:* 10 bd Thomas Gobert 91100 Palaiseau

Lieu du stage / *internship place*: C2N

Titre du stage / *internship title*: Simulation of hot carriers by using ab-initio parameters for energy harvesting.

Résumé / *summary*

Nowadays, energy conversion devices are mainly designed by using macroscopic models (such as the drift-diffusion and the heat Fourier's formalisms) which assume local equilibrium and simplified material properties (energy dispersion, relaxation times…) that must be known a priori.

In the framework of future generations of **energy converters that will most probably involve high energy carriers,** out-of-equilibrium carrier distributions and complex band structures as well as strong quantum effects [1,2], these tools reach their limit of accuracy [3].

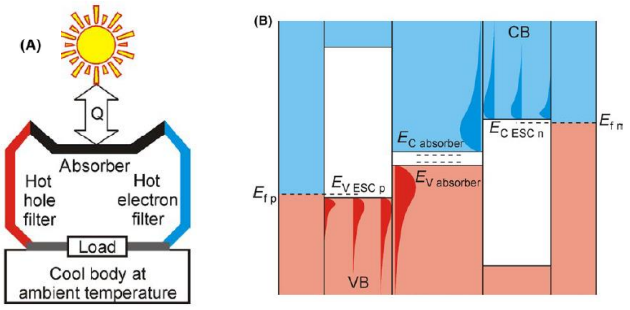

Figure 1: A) Hot carrier solar cell as thermoelectric device. B) Energy bands in hot carrier solor cell from [4].

Besides, these new routes of development will require to investigate a **large panel of new materials** [4] **and nanostructures** probably different from those which are well known and commonly used today in the microelectronics industry such as 2D materials (mono or multilayers). In recent years, a **spectacular progress in *ab-initio* DFT** (density functional theory)-based description of the electronic and thermal transport has been achieved and this method can be used to investigate these recently studied materials.

The goal of this internship proposed in the COMputational electronICS group at the C2N is to developed transport simulation of charge and heat by coupling existing simulation platform [5] with parameter calculated by using ab-initio methods. More precisely, in our home-made Monte Carlo simulator will be included the full band electron/phonon scattering rates, in particular electron/phonon coupling and impact ionization phenomenon (which is important for hot carriers in small gap materials like InAs) as well as interface transmission. Electrical thermal properties as well as the thermalization time of hot carriers in nanostructures will be investigated and compared with the experiment results. The proposed modeling development will be carried out in close connection with the experimental activities performed by J. Chaste and his co-workers in the C2N.

This work is supported by the ANR project "Placho" and the Labex Nanosaclay via the MACACQU flagship. This internship is expected to be continued in a Phd program.

[1] D. Cakiroglu *et al.*, Solar Energy Materials and Solar Cells **203**, 110190 (2019).
[2] T. Abu Hamed *et al.*, EPJ Photovolt. **9**, 10 (2018).
[3] A. J. Nozik, Nature Energy **3**, 170 (2018).
[4] I. Konovalov and V. Emelianov, Energy Sci Eng **5**, 113 (2017).
[5] B. Davier *et al.*, J. Phys.: Condens. Matter **30**, 495902 (2018).

Ce stage pourra-t-il se prolonger en thèse ? *Possibility of a PhD* **? : YES**

Si oui, financement de thèse envisagé ou acquis / *financial support for the PhD* **?**

Financement acquis / *Secured funding*		Nature du financement */Type of funding*	
Financement demandé / *Requested funding*	*X*	Nature du financement */Type of funding*	*ANR et ED*