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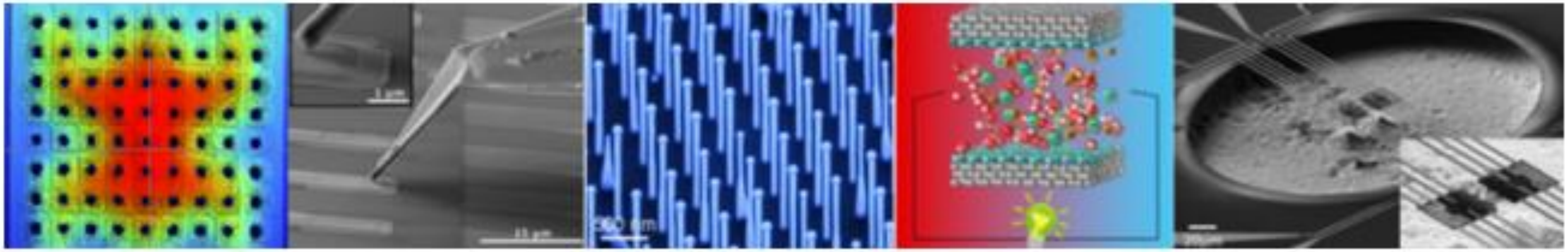
# Poster Pitch

*Oct., 4$^{th}$ 2022*



# Évaluation de l'efficacité inhibitrice des nanoparticles de Fe3O4 contre la corrosion de l'acier au carbone en milieu acide

*Hayette SAIFI*

# Nanocrystalline Zinc Synthesis by Pulsed Current

*Amel BOUKHOUIETE*

# Electron-phonon interaction in semiconductors: coupling of ab initio data for hot carriers with device-oriented simulation methods

*Swarnava MITRA, Raja SEN, Nathalie VAST,*
*Jelena SJAKSTE*

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ELABORATION
MESURES METROLOGIE
SIMULATIONS THEORIE
APPLICATIONS

# Electron-phonon interaction in semiconductors: coupling of ab initio data for hot carriers with device-oriented simulation methods

Swarnava Mitra[1,2], Raja Sen[1], Nathalie Vast[1], and Jelena Sjakste[1]

[1]*Laboratoire des Solides Irradiés, CEA-DRF-IRAMIS, Ecole Polytechnique, CNRS UMR 7642, Institut Polytechnique de Paris, France*

[2]*School of Chemical Sciences, UM-DAE Centre for Excellence in Basic Sciences, University of Mumbai, India*

MaCaCQu

WANNIER90

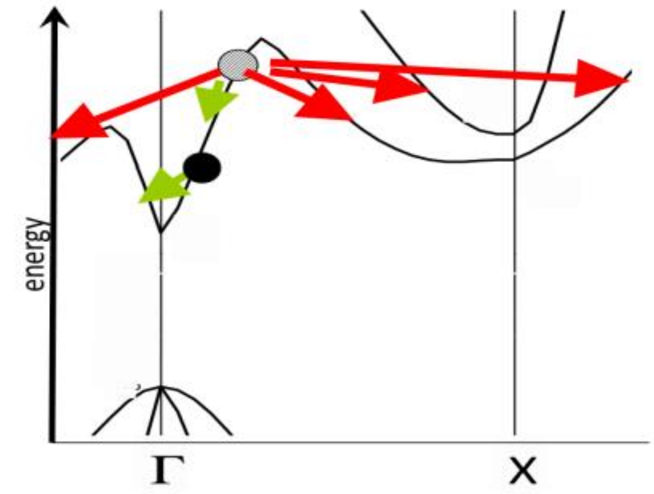
EPW

# Electron-phonon interaction in semiconductors: coupling of ab initio data for hot carriers with device-oriented simulation methods

Electron-phonon interaction $P_{k,k\pm q}^{n,n',\lambda} = \frac{2\pi}{\hbar} |\langle n,k|\Delta W|n',k+q\rangle|^2 \delta(E_{nk'} - E_{nk} \pm \hbar\omega_q^\lambda)$

Ab-initio data:

- Scattering rates and times of individual channels
- Dynamics of Scattering




Hot carriers:

- Dynamics of carrier having excess energy
- Important for photovoltaic (PV)

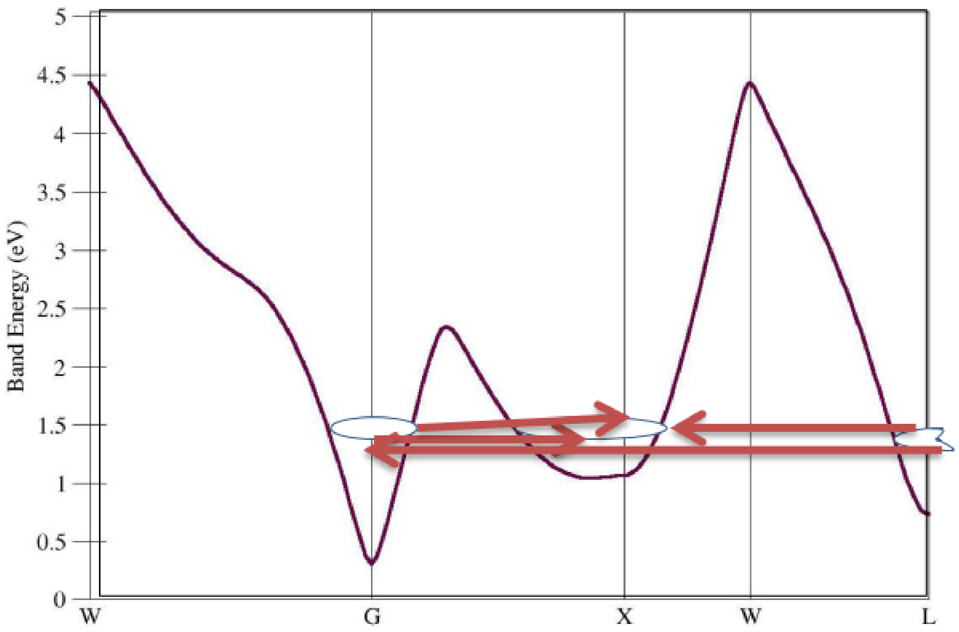
Device oriented simulation methods:

- Stochastic Monte Carlo Simulation
- Calculation of transport properties of hot carriers

**HOW TO COUPLE THE AB-INITIO AND MONTE CARLO?**

# Coupling of Ab-initio and Monte Carlo

Calculation of Deformation Potentials:




- Simple and efficient method using ab-initio
- Intervalley transitions
- Hot carriers
- Feed into the Monte Carlo Simulation

HOPE TO SEE YOU THERE ☺

# Full Band Monte Carlo simulation of phonon transport in GaAs porous nanofilms

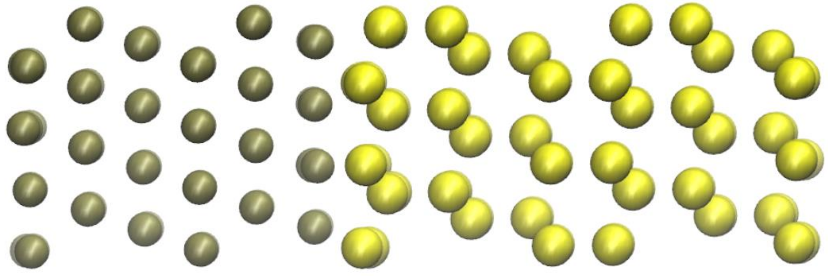
*Junbum PARK, Lorenzo PAULATTO, Marco PALA, Jérôme SAINT-MARTIN*

# Atomistic modeling of interfacial thermal transport across semiconductor-metal interfaces

*Michael DE SAN FÉLICIANO, Christophe ADESSI and Samy MERABIA*

# Atomistic modeling of interfacial thermal transport across semiconductor-metal interfaces

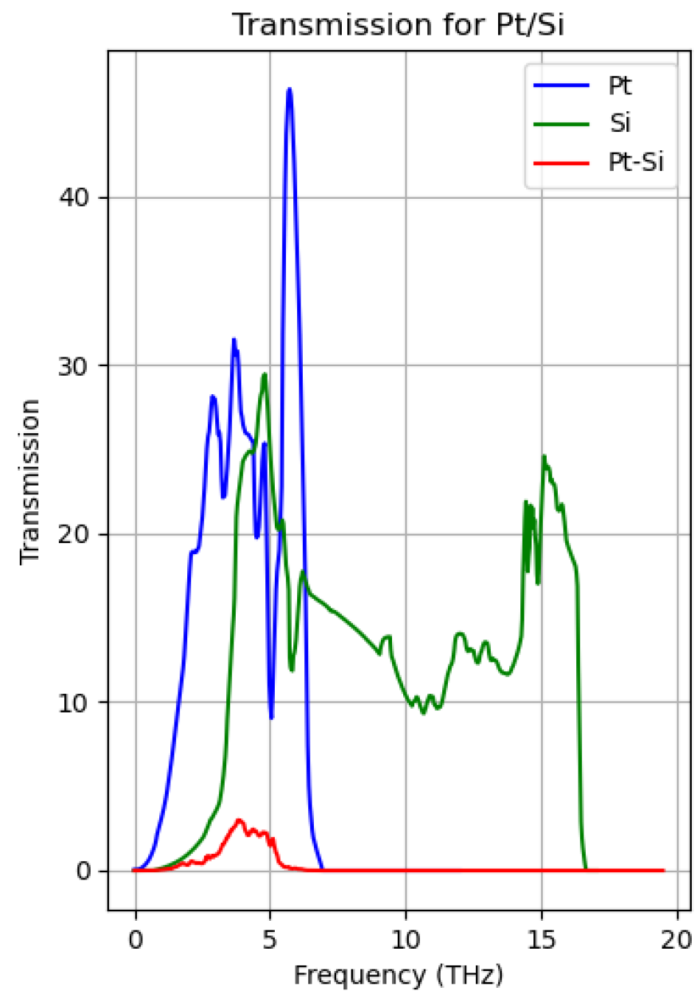
Michael De San Féliciano



With S.Merabia and C.Adessi

# $e^-$(f)ficac $e^-$

- Ab-initio calculations achieved with SIESTA
- Platinum/silicon and gold/silicon interfaces
- NEGF calculations for the transmission and thermal conductance at the interface



# Impact de la matrice polymère dans des dispositifs à base de nanofils de GaN pour des applications de récupération d'énergie

*Amaury CHEVILLARD, Tanbir Kaur SODHI, Elie LEFEUVRE, Laurent COURAUD, Xavier LE ROUX, Laurent TRAVERS, François JULIEN, Maria TCHERNYTCHEVA, Noelle GOGNEAU*

# Impact de la matrice polymère dans des dispositifs à base de nanofils de GaN pour des applications de récupération d'énergie

Amaury Chevillard, Tanbir Sodhi, Elie Lefeuvre, Laurent Couraud, Xavier Leroux, Laurent Travers, François H. Julien, Maria Tchernycheva, Noëlle Gogneau

Financement :
Projet ANR Piezosens
Projet NanoSaclay NanoVIBES

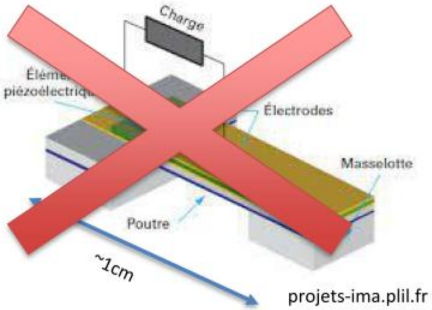
# Contexte et objectifs

Réduction de la taille et consommation de composants électroniques

manomano.fr

alibaba.com

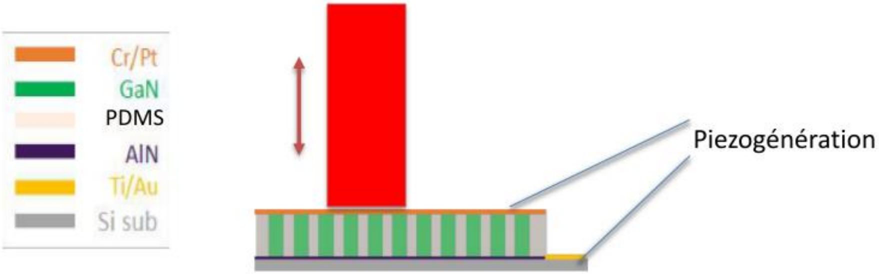
Récupération d'énergie ambiante, par exemple par piézoélectricité




projets-ima.plil.fr

Nécessité de repenser les piézogénérateurs

Nouveau type de piézogénérateur : dispositif à nanofils

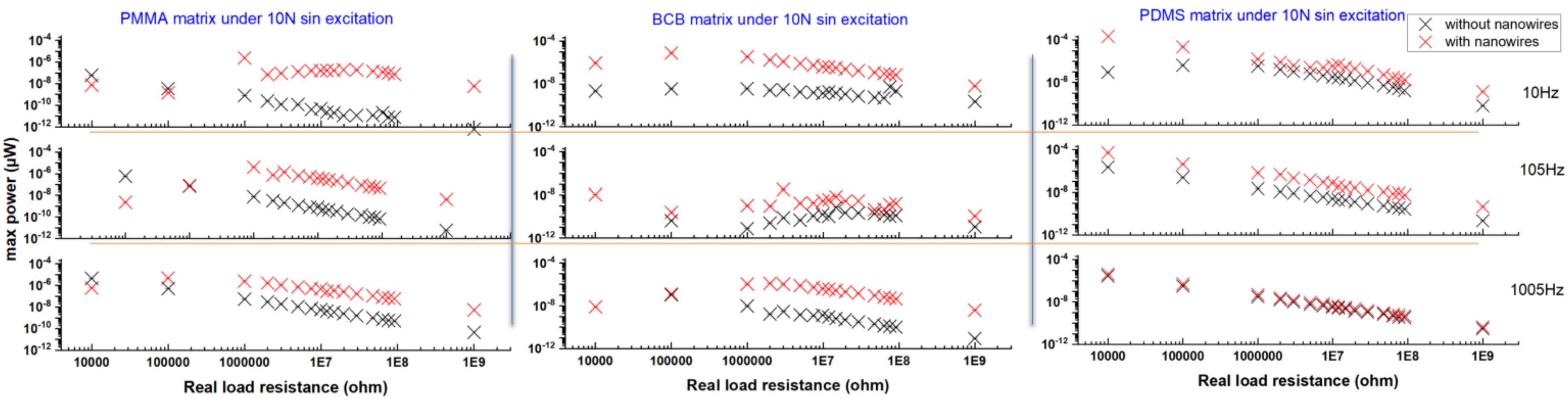



Thèse Lu Lu (2018)

Design du dispositif en fonction de l'application

# Impact de la matrice polymère sur la récupération d'énergie, en configuration capacitive

Conditions environnementales (10N sin excitation, fréquences envorinnemantales)




PMMA : 2.9 GPa

BCB : 2.7-3.1 GPa

PDMS : 0.5-4 MPa

- Réponse électromécanique même sans nanofils
- Le coefficient piézoélectrique $d_{33}$ dépend du composite nanofils+matrice
- La matrice a un impact sur les effets de charges de surfaces des nanofils

# Simulation of the linear and nonlinear response to an electrical excitation in a thermoelectric network using Spice

*Mahdi-Amine MAMOUNI, Christophe GOUPIL, Philippe LECOEUR*

# SIMULATION OF THE LINEAR AND NONLINEAR RESPONSE TO AN ELECTRICAL EXCITATION IN A THERMOELECTRIC NETWORK USING SPICE

M-A. MAMOUNI[1,2] , CH. GOUPIL[1] , PH. LECOEUR [2]

[1]Center for Nanoscience and Nanotechnology (C2N),CNRS, Université Paris-Saclay, 91120 Palaiseau, France
[2]Laboratoire Interdisciplinaire des Energies de Demain(LIED), CNRS UMR 8236,Université Paris-Cité, 5 Rue Thomas Mann, F-75013 Paris, France

# PYDYCO SIMULATOR: SIMULATING THERMOELECTRICITY

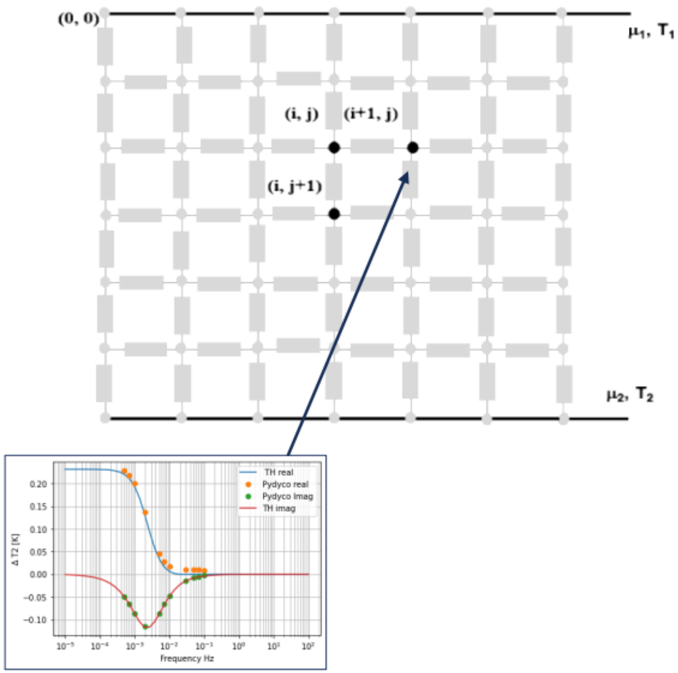



**Fig -** Example of 11x14 network simulated in PyDyCo and the result expected.

**Overview:**

- A solver, written in Python with the exploitation of Spice kernel, following the nodal description of thermoelectricity.
- Simulation of $n \times m$ sized network with heterogeneous structure and different physical properties.
- Taking into consideration the nature of the boundary conditions of temperature, and electrochemical potential.
- The simulation can be either static or harmonic.

**We present:**

- The simulation of an E-type thermocouple response to harmonic electrical excitation, linear and nonlinear response and we compare them to the analytical expressions in the literature.

# Systèmes hybrides photovoltaïques-thermoélectriques pour la récupération d'énergie solaire

*Guilhem ALMUNEAU, Jean-Baptiste DOUCET, Sébastien HANAUER, Inès Massiot, Adnen MLAYAH, Christophe CANDOLFI, Soufiane EL OUALID, Francis KOSIOR, Bertrand LENOIR, Philippe MASSCHELEIN, Mashiul HUQ, Slavisa JOVANOVIC, Philippe POURE, Etienne TISSERAND*

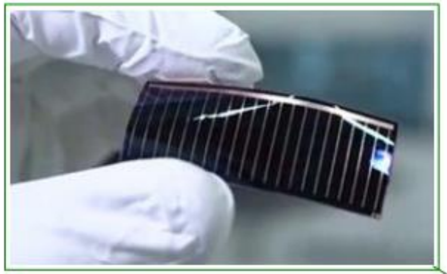
# Hybrid photovoltaic-thermoelectric systems for solar energy harvesting

Project ANR Hydres

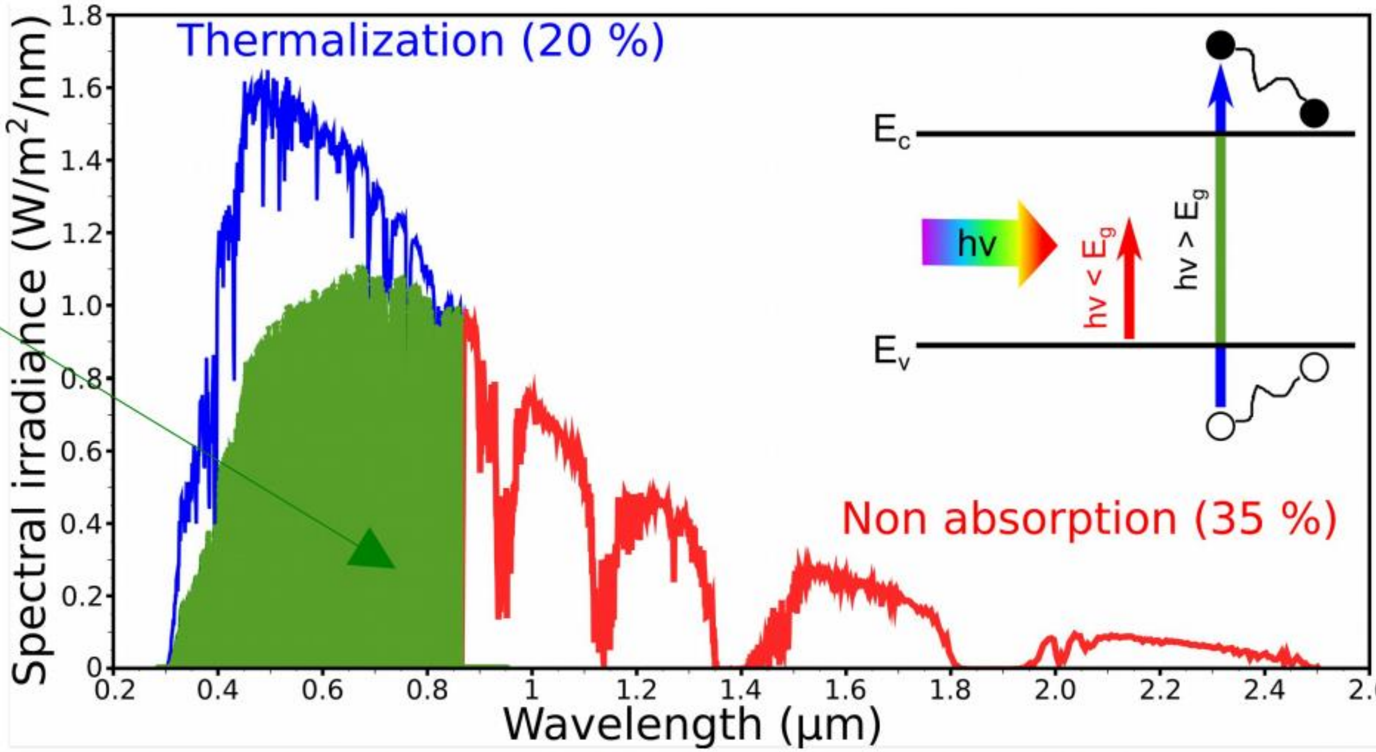
Project leader : Inès Massiot – LAAS-CNRS

# Hydres in a nutshell: motivations

> How to exceed the efficiency limit for a single-junction solar cell ?



GaAs 29,1 %




> Our approach: **photovoltaic-thermoelectric hybridization**

> Targeted application: self-powered microsystems.

# Hydres in a nutshell: objectives & methodology

Project funded by the ANR: **Hy**bri**d** photovoltaic-the**r**moelectric for solar **e**nergy harve**s**ting (2022-2025).

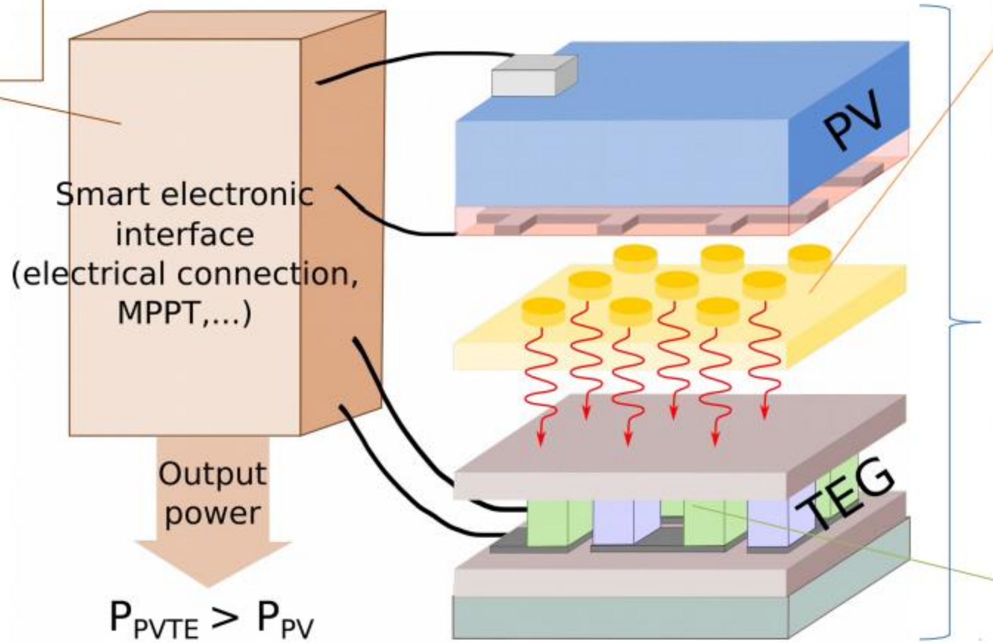
Ultimate goal: **+8-10% absolute gain** with respect to the PV cell at ambient T

> Methodology:

- **Global approach** of the hybrid PV-TE system
- Design & fabrication of **custom building blocks** of the system
- **Multidisciplinary study**
  - Photovoltaics & plasmonics [LAAS-CNRS]
  - Thermoelectrics [Institut Jean Lamour]
  - Smart electronics [Institut Jean Lamour]

# Hydres in a nutshell: scientific objectives

**Model of the complete system** including PV-TE interface + electronic interface




**Plasmonic photothermal antennas** to boost the TEG efficiency

**Technological fabrication process for high thermal coupling**

**Design & fabrication of custom TEG**

# Manipulating heat flows with an electric field

*Lucile FEGER, Fabien GIOVANNELLI, Guillaume F. NATAF, Isabelle MONOT-LAFFEZ*

# Near-field thermophotonic refrigerator: a numerical study

*Thomas CHATELET*

# A novel structure of Cooling Nano-devices: The Quantum Cascade Cooler

*Guéric ETESSE, Marc BESCOND*

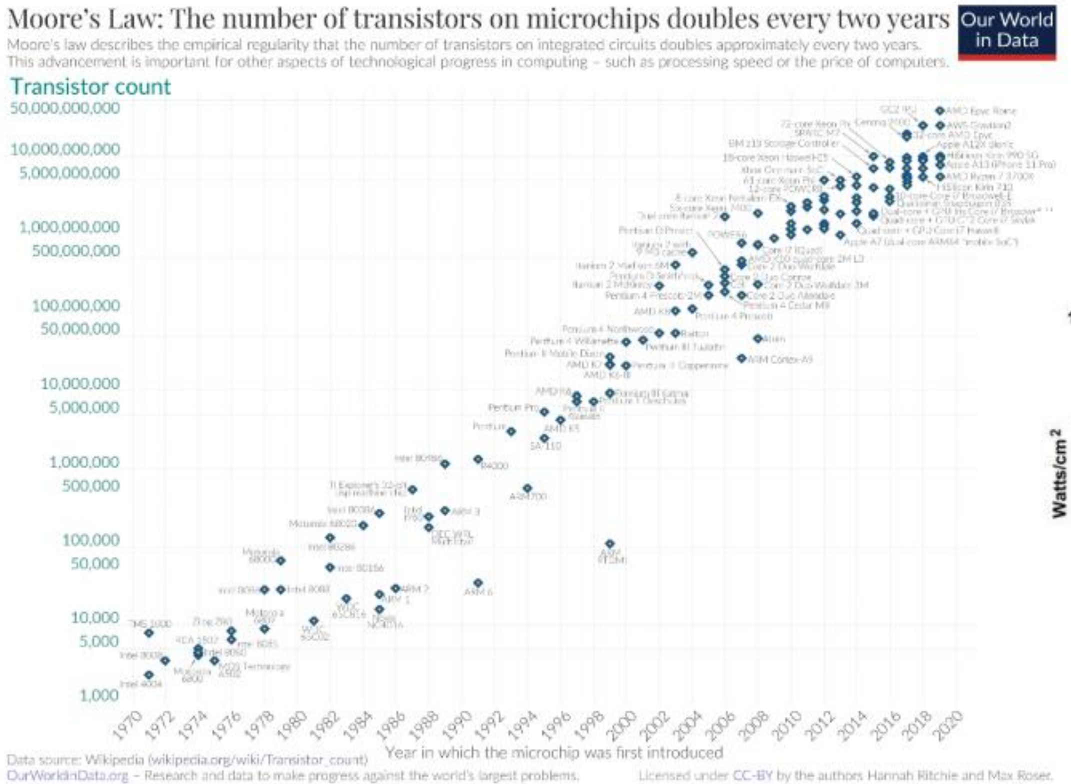
Institut Matériaux Microélectronique
Nanosciences de Provence

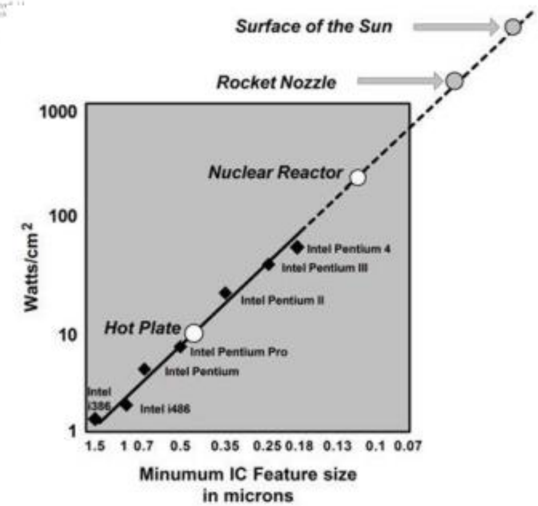
# A novel structure for Cooling Nano-devices: The Quantum Cascade Cooler

Guéric ETESSE
Marc BESCOND

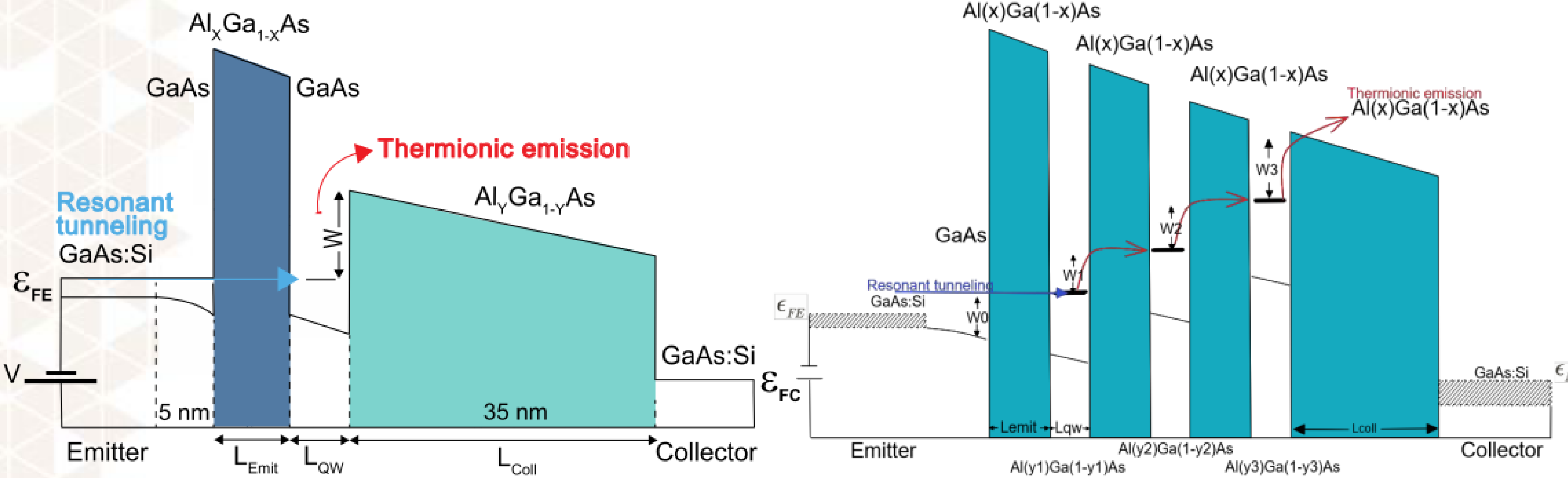
Collaborators: Kazuhiko Hirakawa, Xiangyu Zhu, Chloé Salhani

# The need for new cooling devices:



# Cooling nano-devices based on thermionic emission:

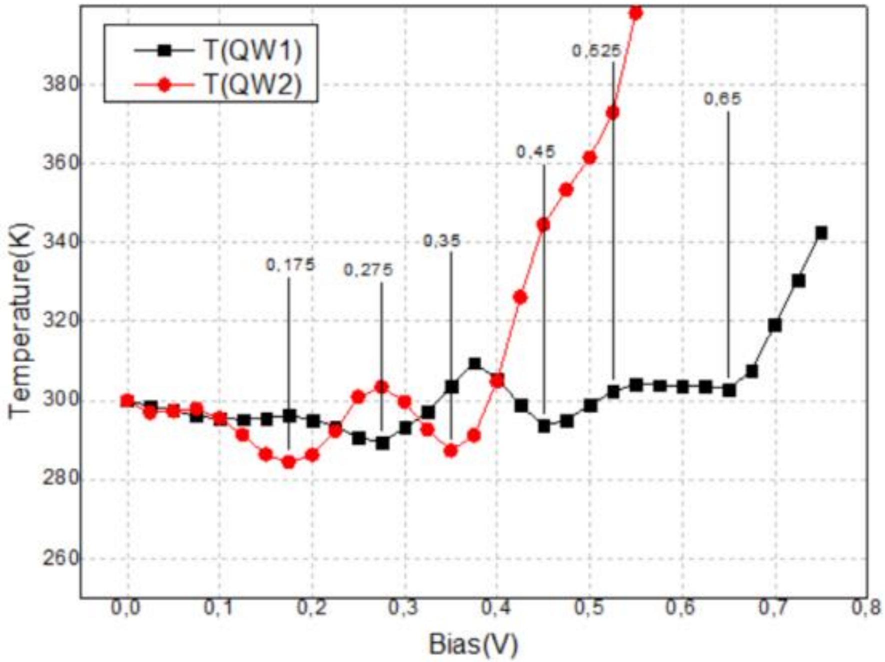


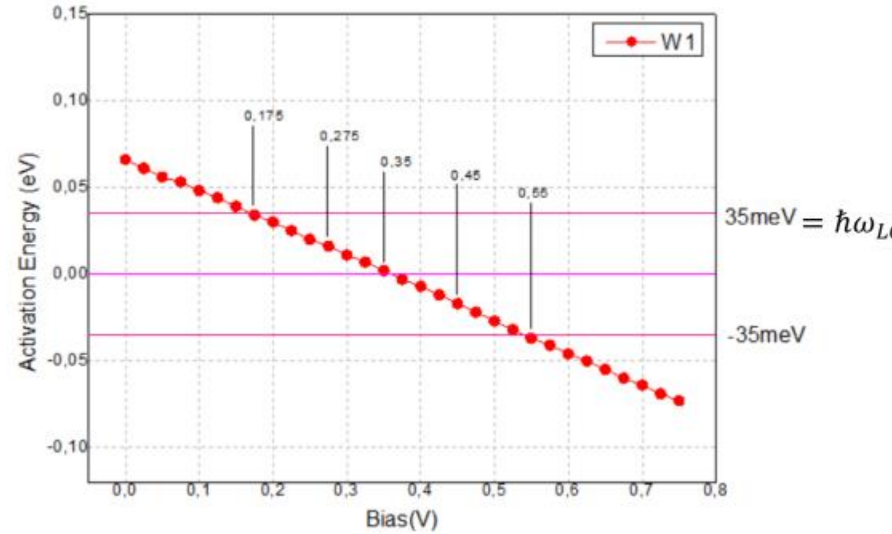

[1]M.Bescond et al. J. Phys.: Condens. Matter 30, 064005 (2018).

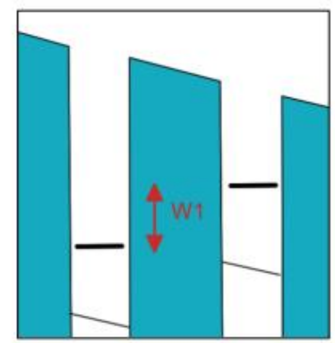
Key message :

- Injecting cold electrons by resonant tunneling and extracting hot electrons by thermionic emission ⇒ Cooling

# Temperature oscillations :




Key message :

- Average electron temperatures inside the are oscillating
- These oscillations depend on the activation energy W1

# Etude de cellules solaires InGaAsN/GaAs en environnement radiatif spatial

*Maxime LEVILLAYER, Sophie DUZELLIER, Thierry NUNS, Christophe INGUIMBERT, Corinne AICARDI, Stéphanie PAROLA, Alexandre ARNOULT, Guilhem ALMUNEAU, Laurent ARTOLA*

# Study of InGaAsN/GaAs solar cells in space radiative environment

Maxime LEVILLAYER[1,2], Sophie DUZELLIER[2], Thierry NUNS[2], Christophe INGUIMBERT[2], Stéphanie PAROLA[3], Alexandre ARNOULT[1], Corinne AICARDI[4], Laurent ARTOLA[2], Guilhem ALMUNEAU[1]

[1]LAAS-CNRS Toulouse, [2]ONERA Toulouse, [3]IES-Univ. Montpellier, [4]CNES

# Context

> How to improve the MJSC efficiency with InGaAsN ?
- Replacing Ge as the bottom cell : **GaInP/GaAs/1eV**
- Adding a 4th junction :**GaInP/GaAs/1eV/Ge**

> Interest for space applications ?
- Key parameter : W/Kg
- **Radiation hardness**

> **Good candidate = 1 eV bandgap InGaAsN lattice matched on GaAs**

# Main results (M. Levillayer PhD work 2018-2021)

> **Optimization of Molecular Beam Epitaxial growth**

- Bulk and 1-junction solar cells with InGaAsN PIN absorber
- Influence of growth parameters (V/III, temperature) on PL, EQE and Light IV chracateristics

> **Degradation study of solar celles under ions radiations**

- Irradiation campaigns **(Electron and proton)** led in ONERA platform in Toulouse
- Evolution of electric and optical properties before, during and after radiation experiences
- Different behaviours on GaAs and InGaAsN
- Studies on single and tandem III-V solar cells

> **Comprehensive study on InGaAsN based solar cells for space PV applications**