Research Internship for 2021

Laboratory:
Centre de Nanosciences et Nanotechnologie (C2N),
CNRS/Université Paris-Saclay

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Theoretical study of thermoelectric properties of 2D materials

Scientific Context

Effective thermal management and energy harvesting become critical issues to improve the sustainability of our electrical energy consumption. Thanks to their unique electrical, mechanical and thermal properties, nanostructures based on 2D materials [1] are expected to increase the energy efficiency of electronic devices.

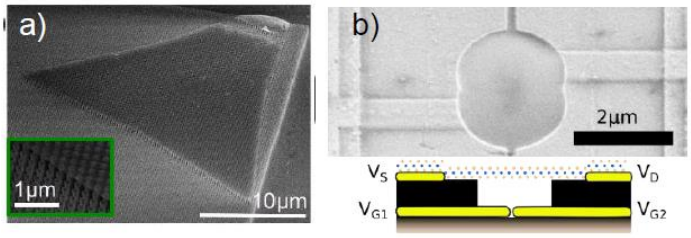

Fig. 1: a) E-beam image of suspended monolayer MoS 2 on array of nanopillars obtained at C2N. b) another geometry of suspended MoS2 with drums geometry with integrated electrical contact. (Courtesy of J. Chaste)

On one hand, active thermoelectric materials that can recycle wasted energy in electronic circuits must have low thermal conductivity and high electrical conductivity. Unfortunately, due to the Wiedemann Franz law, such behaviors are antonymic in common bulk materials, but should be achieved in nanostructured systems [2]. On the other hand, for thermal management (TM) of heat in excess (to be recycled or discharged), materials having as high thermal conductivities as possible are required. The optimization of TM or TE systems based on 2D nanostructures which are smaller than the mean free path of charge and heat carriers requires an accurate understanding of non-equilibrium thermal transport. Thus, specific experimental setup and advanced numerical models must be designed.
This internship is focused on the numerical aspects in the framework of the flagship project MACQCAQU belonging to the NanoSaclay LABEX. However, this work will be performed in strong relationship with the experimentalists involved in the project.

Methodology and Objectives

The objective of this work is to perform a numerical study of the thermal and thermoelectric properties of several 2D materials and their heterostructrures by focusing on non-equilibrium transport phenomena, geometric effects and electron-phonon coupling. Among the 2D materials, layered MoS_2 will be studied first because it is well known in the literature, and then SnS_2 for its promising TE properties.

First, *ab-initio* calculations based on the density functional theory (DFT) will be performed to calculate both the electron and phonon dispersions using the Quantum Espresso software. Then, phonon transport will be studied using a homemade code based on Non Equilibirum Green's Function (NEGF) formalism [3, 4] using a dynamic matrix extracted from DFT. Different types of 2D nanostructures will be evaluated in terms of thermal and thermoelectric properties.

Skills learned

The student will acquire a broad range of skills: in solid state physics (band structure, phonon, electron quantum transport, electron-phonon interaction), technology devices, and scientific computing (DFT software) and programming (Fortran and / or C / C + +, Matlab).

Besides, the results that would be obtained during this internship could be easily published in scientific journals. This work could be a relevant preliminary step for a PhD thesis in our group.

Candidate's Profile

Candidates must have a MSc in Physics, Electronics, Materials Science or related disciplines. We are seeking creative and highly motivated individuals well trained and skilled in scientific research, and available to collaborate in an interdisciplinary team. Programming experience is also desirable, but not mandatory.

Please join a CV, a list of courses that you have followed and results of exams in the framework of your master program, and any other information that you judge useful.

References:

[1] Wang, Y.; Xu, N.; Li, D.; Zhu, J. *Thermal Properties of Two Dimensional Layered Materials*. Adv. Funct. Mater. 2017, **27** (19), 1604134. https://doi.org/10.1002/adfm.201604134.

[2] Principi, A.; Vignale, G. *Violation of the Wiedemann-Franz Law in Hydrodynamic Electron Liquids*. Phys. Rev. Lett. 2015, **115** (5), 056603. https://doi.org/10.1103/PhysRevLett.115.056603.

[3] VT Tran, J Saint-Martin, P Dollfus, S Volz, *Optimizing the thermoelectric performance of graphene nano-ribbons without degrading the electronic properties,* Scientific reports **7** (1), 1-11, 2017 doi.org/10.1038/s41598-017-02230-0

[4] M. Pala, P. Giannozzi, D. Esseni, *Unit cell restricted Bloch functions basis for first-principle transport models: Theory and application*, Physical Review B 102 (2020), 045410. https://doi.org/10.1103/PhysRevB.102.045410