Research Grants for PhD students from the China Scholarship Council

Information Form (please read the guidelines carefully on the website www-csc.utt.fr)

Supervisor's name : TERMENTZIDIS Konstantinos Given names :

Status (prof., assistant prof., …) : CNRS Research Director

Laboratory :	CETHIL	Website address : https://cethil.insa-lyon.fr/
Institution :	INSA of Lyon	Website address : https://www.insa-lyon.fr/

Scientific competence of the supervisor:

Atomistic Simulations: Molecular Dynamics, wave packet propagation
Nanomaterials and Nanostructures: Nanowires, 2D materials, nanofilms, phononic crystals, nanocomposites, solid/liquid nanohubrids, nanoarchitectured materials. liquid/solid nanocomposites
Properties: Thermal and structural properties.
Phenomena: Nanoscale Heat Transfer, beyond Fourier thermal transport: ballistic and quasi-ballistic heat transport, phonon collective effects, thermo-hydrodynamics, phonon interference and diffraction.

Two major publications in the field proposed for the PhD :

1. G. Wiederrecht et al, "Nanomaterials and Sustainability", ACS Energy Lett. 8, 8, 3443 (2023), doi.org/10.1021/acsenergylett.3c01303
2. P. Xiao et al, "MoS2 phononic crystals for advanced thermal management", Science Advances 10, 13, eadm8825 (2024) DOI: 10.1126/sciadv.adm8825

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Description of the research work proposed for a PhD ***Topic # (see list) :*** IV-6. Calculation o

Title : Simulations of thermal properties of novel 1-2-3D nanomaterials based on graphene allotropes

Subject :

The thermal conductivity in nanostructures and nanosctructured materials depends strongly on size and the presence of interfaces, defects, doping, native oxides, amorphisation etc. In these materials, new exotic phenomena beyond the diffusive Fourier law have been observed recently. 2D materials offer an opportunity to examine and to tune these exotic phenomena. On the other hand, the rapid evolution of the elaboration of materials allows us to produce a variety of graphene allotropes as biphenylene, diamene, etc and even to combine them.
The aim of the current PhD thesis is to study by the use of atomistic simulations the thermal properties of nanoarchitectured materials based on different 2D graphene allotropes. These allotropes will be studied seperately or combined in one nanostructure with purpose to examine and design materials with tailored thermal properties. The PhD candidate will be fully incorporated into the MiNT group of CETHIL laboratory at INSA of Lyon, offering a unique opportunity to interact with French national, European and International teams working on Micro and Nano thermal transport.
Applicants need to have a solid base in Engineering, Physics, Nanotechnology or Material Science and good programming skills. The knowledge of Molecular Dynamics Simulations is not mandatory, nevertheless priority will be

Keywords :

2D materials, thermal conductivity, wave propagation, molecular dynamics, beyond Fourier
Computational Materials Science, Condensed Matter Physics, Nanotechnology

Expected collaborations :

French national collaborations: ILM (V. Giordano, S. Merabia, V. Lysenko), LEMTA (D. Lacroix, M. Isaiev), IJL (N. Stein)
International collaborations: Univ. Aristotle of Thessaloniki GREECE (J. Kioseoglou, K. Papagelis), RPI USA (P. Keblinski), UAB SPAIN (X. Alvarez), NSCR GREECE (X. Zianni)

Background required from the applicant :

Applicants need to have a solid basis in Engineering, Physics, Nanotechnology or Material Science.
Background in thermal transport, molecular dynamics and programming (fortran, unix) are a plus but not mandatory.

Existence of a PDF file detailing the proposal ("yes" or "no") : yes
(see guidelines on the website www-csc.utt.fr)