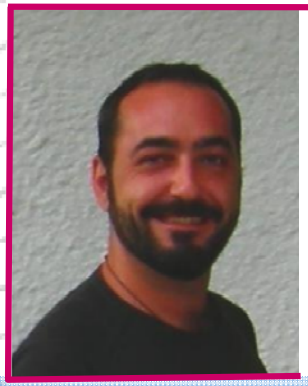
Σ Ε Μ Ι Ν Α Ρ Ι Ο

Thermal Transport Simulations at the Nanoscale

Δευτέρα 12.06.2017
στις 10:00
Αίθουσα συνεδριάσεων
και τηλεδιασκέψεων
του Τμήματος Φυσικής
4ος όροφος



Dr Konstantinos TERMENTZIDIS
Researcher
LEMTA laboratory - CNRS
Nancy, France

Abstract

Understanding and controlling the thermal properties of nanostructured materials and devices are of great interest in a large scope of contexts and applications: biology and medicine, aerospace, communications, computers, electronics and energy applications. The behavior and reliability of these devices strongly depend on the way the system releases heat, as excessive temperatures or temperature gradients result in their failure. A predictive theory for the thermal conductivity assessment is essential for the design of new materials. This is particularly true for example in efficient thermoelectric devices and in micro and nanoelectronics. The correlation between grain boundaries, interfaces and surfaces and the thermal transport properties is a key point to design materials with tailored properties and systems with a controlled behavior.

During this seminar, a number of examples of thermal transport properties obtained by Molecular Dynamics (MD) simulations will be given (nanowires, superlattices, nanoporous materials). The common feature of these systems is that their characteristic system sizes and the phonon mean free path are of the same order of magnitude, which leads to a ballistic heat transport. Furthermore, when the density of interfaces gets large, the energy transport properties of the materials cannot longer be described solely by the thermal conductivities of the constituents of the material, but depend also on the thermal boundary resistance which measures the transmission of phonons across an interface. In this context, molecular dynamics was proven to be a very useful technique to study heat transport in nanostructured materials.