DRF: Thesis SL-DRF-19-0533

RESEARCH FIELD

Solid state physics, surfaces and interfaces / Physique de l'état condensé, chimie et nanosciences

TITLE

Theoretical study of coupled electronic and heat transports to design thermoelectric materials at ambient temperature

ABSTRACT

Thermoelectricity have proven to offer a viable solution for the generation of electrical power (Seebeck effect) and to the problem of overheating in nanodevices (Peltier effect). New technological and scientific efforts are needed to find low-cost efficient materials that will develop the use of thermoelectric devices working at ambient temperature. Numerical simulations, which are the heart of this Ph.D. subject, provide a highly valuable tool to reach this end.

The theoretical method that will allow the prediction of the effect of nanostructuring on the figure of merit ZT will be developed and an integrated simulation tool to evaluate both the diffusive and the phonon-drag contributions to the Seebeck coefficient i.e., the contribution due to electron-phonon coupling, will be provided. This fully ab initio approach will be applied to germanium (abundant and non-toxic) and bismuth (among the material with the highest Seebeck coefficient), achieving a parameter-free description of thermoelectricity for these materials, their nanostructures and their compounds (Si-Ge alloys and Bi_2Te_3).

The BTEs (Boltzmann transport équations) for the electronic and the phonon system, coupled through electron-phonon interaction, will be solved beyond standard approximations. The phonon-phonon anharmonicity and the phonon scattering with surfaces and interfaces in nanostructures will be taken into account, with the aim of tayloring the phonon system to increase the thermoelectric effect.The electron-phonon coupling will be computed with a recent method based on the interpolation in the Wannier space. Finally, the DFT-based results for the electron-phonon coupling will be coupled to a Monte Carlo transport code, opening the

possibility to model even complex nano-devices based on the materials that will be theoretically studied.

LOCATION

Institut rayonnement et matière de Saclay
Laboratoire des Solides Irradiés
Laboratoire des Solides Irradiés
Place: Saclay
Start date of the thesis: 01/10/2019

CONTACT PERSON

Nathalie VAST
CEA
DRF/IRAMIS/LSI/LSI
IRAMIS/LSI
Ecole Polytechnique

91120 Palaiseau
Phone number: +33 1 69 33 45 51
Email: nathalie.vast@polytechnique.edu

UNIVERSITY / GRADUATE SCHOOL

Interfaces: Approches interdisciplinaires / fondements; applications et innovation

FIND OUT MORE

https://www.polytechnique.edu/annuaire/fr/users/nathalie.vast
https://portail.polytechnique.edu/lsi/fr/recherche/theorie-de-la-science-des-materiaux

THESIS SUPERVISOR

Nathalie VAST
CEA
DRF/IRAMIS/LSI/LSI
IRAMIS/LSI
Ecole Polytechnique
91120 Palaiseau