SCIENCES SORBONNE UNIVERSITÉ

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Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
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Director: Guillaume Fiquet

Title: Quasi Harmonic Approximation breakdown: consequences for the thermal transport at extreme conditions

Keywords: Density Functional Perturbation theory, Thermal transport, High pressure, High temperature, Phonon's dispersions, anharmonicity, Inelastic X-rays Scattering

Scientific description: Various recent studies pointed out the inadequacy of a quasi-harmonic approach to correctly describe the lattice dynamics of materials, in particular under extreme conditions, and to account for related properties such as reflectivity, thermal expansion or thermal conduction. A synergetic approach combining experiments and advanced ab-initio calculations is therefore necessary to improve current understanding of the complex phenomena that control the anharmonic properties of materials.This topic is not only of fundamental interest, but also has direct applications, as phonons play a major role for electric and heat transport as well as for superconductivity.

Most advanced theoretical and numerical approaches allow the simulation of anharmonic-controlled phenomena, such as phonon lifetimes and lattice-driven thermal conductivity [S. Baroni et al., Rev. Mod. Phys. 73, 515 (2001)., L. Paulatto et al., Phys. Rev. B 91 (5), 054304 (2015)]. However, macroscopic quantities, such as thermal conductivity or thermo-electric figure of merit ZT, depend on the full phonon spectrum and are very sensitive to the approximations used in the ab-initio simulations and to the specific characteristics of actual materials (degree of crystallinity, presence and nature of defects etc.), which make necessary the direct experimental validation. Thus, within this contest, we propose to study the anharmonic phonon dynamics of the rock-salt compound MgO, by density functional theory calculations, using the Quantum-ESPRESSO code, implementing phonon-phonon interactions up to the third and fourth orders [L. Paulatto, et al. Phys.l Rev.B 87 (21), 214303 (2013), P Giannozzi, et.al. J. Phys.: Condens. Matter 29 (46), 465901 (2017)]. The theoretical results will be directly compared to the relevant experimental quantities already obtained by dedicated infrared and x-ray spectroscopy techniques. In particular we will compute the phonon energy and lifetime in the whole Brillouin zone as a function of pressure and temperature, together with the expected measured spectral density functions $\sigma(\boldsymbol{q}, \omega)$ and the final states involved in the major decay processes [Giura et al. Phys. Rev. B 99, 220304(R) (2019)]. An improved knowledge of all the decay channels, and how these are affected by external parameters such as pressure and temperature, will allow the accurate determination of the phonon lifetime and consequently the correct treatment of the thermal transport.

Techniques/methods in use: Density Functional Perturbation Theory, Inelastic X rays Scattering
Applicant skills: Solid basis in quantum physics and condensed matter physics, knowledge of computational methods, motivation for theoretical modelling, curiosity for experimental investigations and methods.
Industrial partnership: N

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Possibility for a Doctoral thesis: Y : Ecole doctorale ED397, ED564 (ED PIF)