

Title : Electron and phonon dynamics in photoexcited solids**Supervisors :** B. Arnaud and R. Busselez**Phd thesis project**

Pump probe experiments like optical pump probe experiments, time resolved X-ray diffraction, or time resolved photoemission experiments are currently used to study electron and phonon dynamics in nanostructures on time scales ranging from a few femtoseconds to a few picoseconds. Among the aforementioned techniques, optical pump probe experiments have evolved to an advanced degree and are daily harnessed in the NOVA group to study the mechanisms of coherent phonon generation or even the possibility to demagnetize a sample with an ultrashort laser pulse. It is often difficult to interpret experimental results without resorting to models whose parameters can be inferred from *ab-initio* calculations. There are few calculations because of the need to describe non-equilibrium phenomena occurring on different time scales and length scales. Nonetheless, *ab-initio* calculations combined with models already shed new light on ultrafast physics, especially on the coherent phonon generation[1], on the non thermal melting processes[2] or on the energy transfer from the electronic degrees of freedom to the vibrational degrees of freedom[3].

This theoretical Phd thesis includes four parts where *ab-initio* calculations and models are involved :

(1) The study of the mechanisms of coherent optical generation in a topological insulator (Bi_2Te_3), which is currently investigated in the NOVA group[4, 5]. The mechanisms of coherent optical phonon generation following a THz pump pulse have been partly elucidated but the mechanisms for an optical pump pulse (400 nm) remain to be explored. The main idea is to compute potential energy surfaces for a constrained number of electron-hole pairs in order to confirm or deny an hypothetical displacive mechanism.

(2) The study of the mechanisms of coherent acoustic phonon generation following a THz or an optical pump pulse. The goal of this part is to compute both the thermal and electronic stress from first principles and to solve the elasticity equations in order to predict the shape and amplitude of the strain propagating inside the sample as a function of the energy deposited in the electron system by the pump pulse. The validity of the approach will be ascertained by computing the variation of the transmittivity arising from the generation of acoustic phonons. To achieve such a goal the calculation of the photoelastic coefficients in an approach where excitonic effects are potentially included is mandatory[6].

(3) The study of the mechanisms of coherent acoustic phonon generation in Bi, Sb and As. A first step has been achieved since the thermal stress is well described within the quasi-harmonic approximation for Bi[7] and Sb but not for As. From a fundamental point of view, it's important to understand the reasons for this failure before modelling time-resolved X-ray diffraction experiments.

(4) Development of a tool to compute the effective electron-phonon coupling describing the energy transfer from the electronic system to the ionic system[3]. This tool will benefit from the works about Wannier functions[8], that are useful to interpolate the electron-phonon matrix elements.

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