Title: **Theoretical study of electron-phonon coupling and of carrier dynamics in materials for potential photovoltaic and thermoelectric applications.**

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Research Area: Condensed Matter Physics, Materials Science

Methods: Density functional theory, Density Functional Perturbation theory, Boltzmann Transport Equation, Wannnier interpolation

PhD track subject:

Most of the absorbed solar energy is lost to heat. Is it possible to recover it? How to improve the thermoelectric devices? In solids, the quanta of atomic vibrations are called phonons. Excited electrons lose energy to create phonons. Interaction of excited electrons with lattice vibrations (electron-phonon interaction) plays a central role in nanoelectonics, for optoelectronic devices, photovoltaic and thermoelectric materials.

We propose to study, from the theoretical and computational point of view, the atomic structure, the electronic and vibrational properties, and the electron-phonon coupling in materials of potential interest for photovoltaic or thermoelectric applications.

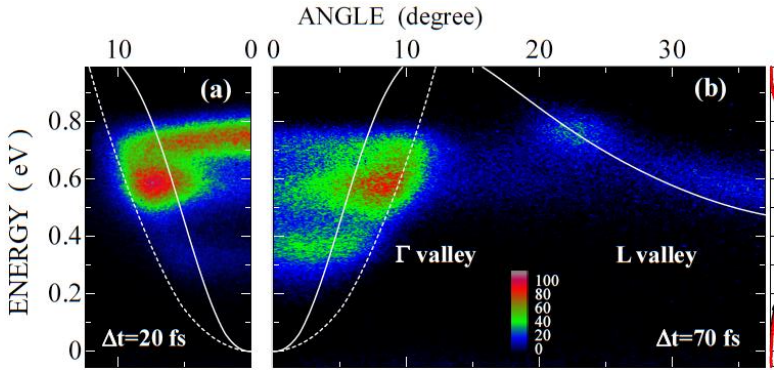

Fig. The evolution in time of the excited electrons in GaAs, measured by photoemission experiment. One can see electrons moving "down" in energy between 20 fs (panel a) and 70 fs (panel b), due to interaction with phonons. Our calculations allow to interpret such experiments.

References:

[1] Chen, Sjakste et al, PNAS 117, 21962-21967 (2020)

[2] J. Sjakste, K. Tanimura, G. Barbarino, L. Perfetti, and N. Vast, Hot electron relaxation dynamics in semiconductors: assessing the strength of the electron-phonon coupling from the theoretical and experimental viewpoints. J. Phys.: Condens. Matter 30, 353001 (2018)