# Carrier dynamics in materials from first-principles

Nicola Bonini
Department of Physics, King's College London

Understanding and modelling carrier dynamics and energy dissipation phenomena in bulk and nanostructured materials is a key issue for the design of high-performance devices for opto- and nano-electronics.
Here we present a first-principles study of carrier dynamics and transport in graphene-based materials and bulk semiconductors. Modelling these phenomena requires an accurate description of the electronic and vibrational properties of these systems, including electron-phonon and phonon-phonon interactions. For this we use density functional theory, and carrier scattering rates are then computed using perturbation theory. Electrical and thermal transport properties are calculated via the exact solution of the Boltzmann transport equation.
Our results provide a detailed characterization of the inelastic relaxation mechanisms that determine the dynamics of charge and heat carriers, of crucial importance to assist the interpretation of spectroscopic measurements. We also discuss the relevance of these findings to model and understand the transport properties of graphene and doped semiconductors.