INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

Dr. Nicola Bonini

Department of Physics, King's College London,
London, United Kingdom

Monday, June 4, 4:30 p.m. ICAMS Seminar room

Thermal and electrical transport at the nanoscale from first principles

Understanding and modelling transport properties and energy dissipation phenomena in nanostructured materials is a key issue for the design of high-performance nanoscale devices. Here we present a first-principles study of transport properties in graphene and in silicon-germanium alloys and superlattices. Modelling these phenomena requires an accurate description of the electronic and vibrational properties of these systems, including phonon-phonon and electron-phonon interactions. For this we use density functional theory, and phonon and electron scattering rates are computed using perturbation theory. The transport properties are then calculated via approximate solutions of the Boltzmann transport equation. Our results provide a detailed characterization of the inelastic relaxation mechanisms and of the relative importance of the individual carriers' scattering processes. We discuss the relevance of these findings to understand the transport properties of graphene and to obtain practical design rules to engineer silicon-germanium nanostructures for thermoelectric and thermal management applications.