# **GRANSPORT:** Correlations and defects in graphene and related materials: Chargeand heat transport

**Main area:** BSR06_Modelling charge and heat transport in GRM - based composites
**Keywords:** graphene; 2D materials; van-der-Waals heterostructures; GRM composites; charge transport; heat transport; 2D elasticity; kinetics; hydrodynamics; plasmonics; superconducting hybrids; analytical methods/models; ab initio; tight-binding simulations; multiscale modeling; electron-electron correlations; defects and impurities; electron-phonon interaction; Moire patterns; far-from-equilibrium phenomena
**Duration (months):** 36
**Total project funding:** € 962.000

## Abstract

The project GRANSPORT aims at developing a global and comprehensive portfolio of realistic modeling tools for studying transport in materials of relevance for technology innovation in Graphene Flagship. Within the Joint Transnational Call 2017 “Graphene”, GRANSPORT will provide a platform for merging analytical and computational approaches to investigate transport properties of complex forms of graphene and related 2D materials (GRM), including their hybrid structures. The consortium consists of renowned groups that all are very active and experienced in the fields of analytical theory, first-principles calculations, mesoscopic transport, and multiscale methods. It will establish a parallel complementary task force and action to support the existing Flagship activities. The key research objectives of the project are as follows: (i) to develop an effective description of graphene and GRM structures, including tight-binding modeling (Kwant) enhanced by Quantum Monte-Carlo and DMRG machinery, hydrodynamic and kinetic-equation description of GRM, and to explore charge and heat transport, correlations, as well as far-from-equilibrium kinetics at the mesoscale; (ii) to investigate the interplay of elastic and transport properties of GRM, applying multiscale modeling to achieve high predictability of theoretical description; (iii) to design and investigate hybrid devices based on GRM and superconductors; (iv) to work out interfaces between nano- and mesoscale computational approaches, including microscopic validation and parameterization of large-scale models and establishing the library of defects and impurities in GRM. By exploring the transport and kinetics from nano- to mesoscale, GRANSPORT will enable conceptually new approach to complex (hetero-) structures to exploit the potential of 2D materials for electronic, plasmonic, photonic, and quantum communication applications. Networking European leaders in advanced quantum simulations and analytical theory will strongly benefit the achievements of priority science and technology goals of Graphene Flagship.

## Consortium

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