

## *Transport in nanostructures. Model and first-principles calculations.*

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### **Introduction**

The enormous interest in graphene, a two-dimensional (2D) honeycomb lattice of carbon atoms discovered in 2004, has both fundamental and practical reasons. The electronic properties of graphene are related to the peculiar nature of its band states in the vicinity of the Fermi level. These states possess a linear dispersion and are described by an effective Hamiltonian formally identical to that of relativistic massless particles (Dirac fermions), albeit with a velocity 300 times lower than the speed of light. This leads to a range of interesting phenomena like finite minimal conductivity, the Klein paradox (i.e. tunneling with no attenuation) and the anomalous quantum Hall effect which can be observed even at room temperatures. The practical interest stems mostly from the fact that carriers in graphene, whose number and character (electrons or holes) can be modified by the field effect, possess exceptionally high mobility. Structures similar to graphene but based on other elements (Si – silicene, Gr -- germanene) are also intensively studied in recent years.

### **Research project objectives and methodologies**

The thesis research will consist of theoretical studies of transport properties of nanostructures, in particular graphene and graphene-like materials. The subject of interest will be in particular the scattering of charge carriers (electron and holes) on lattice defects, impurities, edges, ripples or antidots. The particular attention will be given to the relation between the transport properties and the electronic structure. The calculations will be carried out using model Hamiltonians and/or first-principles (ab-initio) methods.

The candidate will have to master the elements of the solid state theory and theory of transport phenomena. The basic programming skills, or the ability to learn them, will be required.