

THEORETICAL AND COMPUTATIONAL NANOSCIENCES

$$\Psi_p^\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi_p^\pm(A) \\ \Psi_p^\pm(B) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} se^{i\theta/2} \\ e^{-i\theta/2} \end{pmatrix}$$

Led by ICREA Prof. Stephan Roche, the Theoretical and Computational Nanosciences Group theoretically explores exotic quantum transport phenomena in low dimensional structures and complex materials including carbon nanotubes, DNA, graphene, organic crystals and topological insulators. Targets of interest include the investigation of the effect of chemical and topological disorders, as well as electron-phonon coupling and spin-orbit interaction on quantum interferences, localization phenomena, decoherence mechanisms, electromechanical coupling between charges flow and vibrations of systems. Methodological developments target innovative quantum transport approaches to describe charge, spin, phonon, or polaron dynamics in complex matter.

BACKGROUND

The exploration of the nanosciences requires the development of specific theoretical tools to unveil the origin of complex quantum phenomena, strongly driven by the nanoscale chemical complexity of materials and devices, and sometimes out of the reach of experimental inspection. Two research directions for theory are highly challenging. First it is often necessary to tackle quantum (transport) phenomena beyond conventional semiclassical treatments and mean field approaches. Second, there is a crucial need for the development of multiscale computational strategies, keeping the accuracy of state-of-the-art ab initio methods, but allowing the calculation of physical observables in realistic models. These are the challenges that the group aim to tackle, within the context of charge, spin, phonon or polarons dynamics in complex states of matter and low dimensional structures.

RESEARCH ACTIVITIES INCLUDE:

Graphene Electronics and Spintronics.

The goal is to explore the quantum transport properties in chemically and mechanically modified forms of graphene-based materials and devices. This includes the study of mobility gaps, localization phenomena, inelastic transport, decoherence mechanisms and spin-dependent transport features.

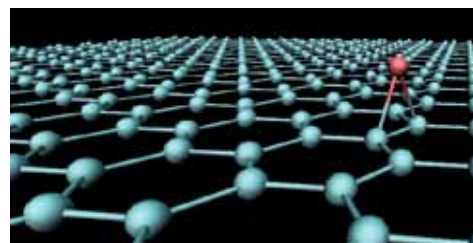
Carbon Nanotubes and Nanoresonators.

The coupling between nanotubes vibrations and transport is investigated, based on the development of innovative approaches combining molecular dynamics and real space transport algorithms (Kubo-Greenwood).

Topological Insulators-TI. The objective of the Group is to develop realistic models of TI, accounting the strong spin-orbit interaction, and to explore the exotic transport properties of surface states in 2D and 3D models, in the pres-

ence of chemical and topological disorders. The assessment of the topological invariance robustness against material imperfections, interface geometries and external influences (field effect, magnetic fields, etc.) is targeted.

Multiscale Quantum Simulation of Nanodevices. The aim is to establish state-of-the-art multiscale simulation methodologies for nanodevices, bridging state-of-the-art first principles methods to compact models in the field of Information and Communication Technologies. This includes the understanding and control of Schottky-Barrier field effects devices, spin-devices and thermoelectrics. All research activities of the group are closely connected to the experimental challenges endeavored at ICN spanning from nanoelectromechanical systems, to nanoelectronics, spintronics and phononics. One key objective of the group also lies in the establishment of a long-term collaborative research strategy with the Theory and Simulation Group headed by Pablo Ordejon at CSIC, within the framework of the CIN2 collaboration.



ICREA PROF. STEPHAN ROCHE
GROUP LEADER

Prof. Stephan Roche studied Theoretical Physics in the Université Joseph-Fourier (UJF) and Ecole Normale Supérieure in France, and then received a Ph.D. in Physics in 1996 working at the French CNRS. After several (postdoc) research stays in Japan (Tokyo) and Spain (under the support of the Japanese JSPS and the European Commission), he was appointed in 2000 as a Professor Assistant at the UJF and then as a Researcher at the Commissariat à l'Energie Atomique-CEA in 2004. The same year, he received the "Habilitation à diriger des Recherches" from the UJF. During his stay at the Institut of Nanosciences and Cryogenics (INAC) of CEA, he was in charge of the coordination of the "quantum simulation platform" of the CHEMTRONICS program, and involved in the preparation of the NANOSIMULATION CEA program. In 2009, he was awarded the Friedrich Wilhelm Bessel prize by the Alexander Von-Humboldt Foundation (Germany) and worked 6 months in Technische Universität Dresden. He is currently ICREA Research Professor and head of the Theoretical and Computational Nanoscience Group of the ICN which focuses on the theoretical understanding of quantum transport phenomena from the molecular to the mesoscopic scales.

