Alliance 8: Theoretical and Computational Physics

Research axes and facilities

The current activity in theoretical and computational condensed matter physics in Grenoble has evolved substantially these last years, thanks to the recent arrival of a number of junior and senior scientists. Our joint activity has many fruitful links to other communities such as applied mathematics, atomic and subatomic physics or geophysics (formalized by the recently created Grenoble Center for Theoretical Physics, CTPG), and with close proximity to many experiments. On the computational physics side, Grenoble has been fostered by the successful coordination, arguably exemplary in France, of the different nodes in the Rhône-Alpes region (CIMENT and CIRA programs).

This "transverse alliance" within LANEF goes from theory based on model Hamiltonians (aiming at capturing the essential physics of complex phenomena) towards full *ab initio* simulations which aim at predicting the properties of real materials. Current activities are in phase with international developments, such as the study of quantum information, carbon nanotubes and graphene, Casimir phenomena, Anderson localization, superconductivity, complex materials such as multiferroics or cold atoms as tools in condensed matter physics, molecular magnetism. Several prospects exist for theoretical work related to energies of the future, with ongoing research aiming at understanding and modelling materials and devices for inorganic, organic and hybrid photovoltaics, thermoelectricity, fuel cells and batteries. This alliance participates actively in an innovative national project on advanced supercomputing as well as in the creation of a local facility to develop large scale parallel numerical software.

Actions within LANEF

The alliance's current projects include:

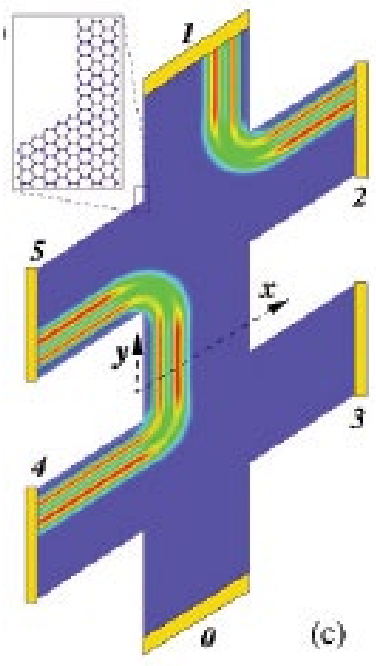
Charge/spin transport. Properties in nanostructured, tailored (doped, defective, functionalized, etc.) materials, tubes, wires, graphene, atomic gazes, magnetic multilayers, Josephson nano-junctions, molecular systems (fullerenes, polymers), with an emphasis on mobility reduction or enhancement by disorder, electronic correlations, electron-phonon coupling, spin control by interaction with magnetic electrodes or molecular magnets, quantum entanglement etc. These activities – supported by many-body techniques, random matrix approaches and ab initio simulations, naturally integrate into Alliances 2 (spintronics and nanomagnetism), and 3 (nanoelectronics). Similar questions and techniques are being explored for thermal energy transport at the nanoscale.

Optical properties of nanostructured inorganic and/or organic systems. Core/shell nanowires (with applications in photovoltaics), molecules on graphene or nanotubes, (dye-doped) semi-conductor powders, gold droplets on Si-surface. Methods used are state-of-the-art many-body techniques (GW, Bethe-Salpeter, optical Bloch/rate-equations) within semi-empirical (large scale) and/or ab initio formulations. Theoretical approaches in nano-photonics and plasmonics (Bloch equations, Green function techniques…) are developed and applied to control electromagnetic fields at subwavelength scales, to optimize antireflection coatings, to model Casimir phenomena and random lasing. These activities have a direct link with Alliance 1 (photonics).

Complex phenomena in systems with competing interactions. Unconventional Iron-based superconductors, frustrated magnets, or multiferroic materials, with potential applications as switches, magnetic field sensors or new types of electronic memory devices. They can be studied using model calculations coupled eventually to ab initio determination of the interactions. These studies are performed in close connection with experimentalists, mostly active in Alliance 5 (Advanced Superconductivity).

Physical modelling of bio-sensors. Based on polymer physics and statistical mechanics, theoretical models for the performance and governing principles of bio-sensors and micro-arrays are being developed and validated by physicochemical experiments, with clear targets in Alliance 7 (nanosensors for healthcare).

Modelling of electrical energy systems. Designing future electrical systems requires either extensive computation in view of their complexity (nonlinear, many degrees of freedom, nondeterministic) or a complete revision of their analytical models. This project aims at creating an active link with Alliance 4 (electrical energy). The broad support to the activities of the experimental groups within the alliance, the building of innovative concepts allowing to "think differently" and the development of state-of-the-art computational tools (GW, Bethe-Salpeter, Non-equilibrium-Green's function techniques, quantum Monte Carlo, HIL), often within widely distributed international packages, are some of the goals that the LANEF project will foster and facilitate in the coming years.



Numerical simulation of edge states in a graphene Hall bar at high magnetic field

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