DIPC PhD OFFER

QuantumChemPhys

Theoretical Chemistry and Physics at the Quantum Scale

Donostia International Physics Center DIPC is currently accepting applications for **one PhD position**. This is a unique opportunity for highly motivated students, recently graduated from University in physics, chemistry or related fields, to start a research career in an international environment. The contract will cover a period of 3 years. Annual salary will be 15.972€/year (before taxes) during the first year, with subsequent smooth increases over the next two.

The research project will be developed in the framework of the Transnational Common Laboratory "***QuantumChemPhys*** *– Theoretical Chemistry and Physics at the Quantum Scale*", built between University of Bordeaux (UBx), University of the Basque Country (UPV/EHU), and Donostia International Physics Center (DIPC). The PhD research project will be co-supervised between a researcher at UBx and a researcher at DIPC-UPV/EHU. During the PhD period, the student is expected to spend some time at each one of the supervising institutions and mobility is therefore required. The PhD degree will be awarded by both UBx and UPV/EHU.

Three possible research projects are detailed below. The successful candidate will have the opportunity to select one among them. The choice can be made either before or after the selection procedure is over.

Interested candidates please send an updated CV including an academic transcript with the obtained marks, a brief statement of interest, and contact information to phd@dipc.org. Reference letters are welcome but not indispensable. The particular PhD project(s) preferred by the candidate may be stated as well. Applicants are advised to hold, or be in the final year of a Master's degree in physics, chemistry or material science.

The review of applications is scheduled on February 29th 2016. Applications will be evaluated by a Committee designed by the DIPC board on the basis of the following criteria (with point weights indicated in parentheses):

- CV of the candidate (60%)
- Adequacy of the candidate's scientific background to the project (20%)
- Statement of interest and reference letters (10%)
- Others: Diversity in gender, race, nationality, etc. (10%)

Evaluation results will be communicated to the candidates soon after. The position will only be filled if a qualified candidate is found.

PROJECT 1.- Dynamical aspects of quantum transport in nano-electronics

Contact persons: Remi Avriller (U. Bordeaux, remi.avriller@u-bordeaux.fr) and Thomas Frederiksen (DIPC, thomas_frederiksen@ehu.eus)

The fundamental limitations to miniaturization of electronics in the semiconductor industry have driven both fundamental and applied research to find new and complementary technological alternatives. Potential candidates for ultimately scaled electronic devices include single molecules [1] and carbon-based materials (e.g., nanotubes, nanoribbons, and graphene) [2] which present unique and tunable electronic and mechanical properties.

In recent years many efforts have been devoted to understand electronic transport in such nanoelectronic devices [1,2,3]. A crucial phenomenon to take into account that limits performance is the coupling between the electronic current (electrons transmitted across the device) and collective modes of atomic vibrations of the junction (phonons) [4]. This interaction can lead to energy dissipation, heating of the junction, mechanical instabilities, and finally to the breakdown of the device. A global understanding of these dynamical aspects between electronic and vibrational degrees of freedom is still lacking.

In this PhD project we plan to develop new theoretical and numerical tools to characterize such effects. Ab-initio methodology based on a combination of density functional theory (DFT) and nonequilibrium Green's functions (NEGF) can shed light on transport characteristics of specific atomic-scale device structures [5], and quantify the impacts of electron-phonon interactions on electronic conductance [6] and current fluctuations (inelastic shot noise) [7]. We will develop these spectroscopic tools further to gain information about the electronic structure, the e-ph coupling strength, and heating effects of actual devices. We also aim at studying current-induced mechanical instabilities and self-oscillations. This will be done with a combination of atomistic simulations and model calculations with the further aim to propose possible ways to experimentally detect such effects. This project thus opens up new perspectives for design and control of atomic dynamics in nanoelectronics.

The project will be supervised by R. Avriller and F. Pistolesi from U. Bordeaux and T. Frederiksen from DIPC. These researchers have complementary expertises in the fields of quantum transport and nanomechanics and previous collaborative experience [7,8]. This project will stimulate new activities between the involved research groups.

[1] S.V. Aradhya & L. Venkataraman, Nature Nanotechnology **8**, 399 (2013)
[2] L. E. F. Torres, S. Roche, & J. C. Charlier, *Introduction to graphene-based nanomaterials: from electronic structure to quantum transport*, Cambridge University Press (2014)
[3] D. Dundas, E. J. McEniry, & T. Todorov, Nature Nanotechnology **4**, 99 (2009)
[4] N. Agrait, A. L. Yeyati, & J. M. Van Ruitenbeek, Physics Reports, ***377***(2), 81-279 (2003)
[5] M. Brandbyge, J. L. Mozos, P. Ordejon, J. Taylor & K. Stokbro, Phys. Rev. B **65**, 165401 (2002)
[6] T. Frederiksen, M. Paulsson, M. Brandbyge & A.-P. Jauho, Phys. Rev. B **75**, 205413 (2007)
[7] R. Avriller & T. Frederiksen, Phys. Rev. B **86**, 155411 (2012)
[8] G. Micchi, R. Avriller, and F. Pistolesi, Phys. Rev. Lett., accepted (2015)

PROJECT 2.- Charge, spin and heat transport in superconducting nanostructures with generic spin fields

Contact persons: F. Sebastián Bergeret (CFM/DIPC, sebastian_bergeret@ehu.eus) and Alexandre I. Buzdin (U. Bordeaux, alexandre.bouzdine@u-bordeaux.fr)

We are looking for a PhD student to work on a cooperative project between the Mesoscopic Physics Group at the DIPC and the Group of Prof. Alexandre Buzdin at the University of Bordeaux.

The PhD student will be offered different topics in the field of quantum transport in superconducting hybrid structures. During the PhD the candidate will be introduced to the quasiclassical technique to deal with spin interactions in superconducting heterostructures. Topological effects in superconductors with strong spin-orbit and spinsplitting effects will be derived and illustrated within this methodology. Also, a nonequilibrium description of superconducting spintronics will be developed. Ultimately, the developed formalism will be applied to concrete situations, specially when charge, spin and heat currents are coherently coupled.

The project will fill a gap in material science, since it will focus specifically on the difficulties to observe topological effects in experimentally accessible heterostructures. In addition, the extended quasiclassic methods will be helpful for the mesoscopic physics community for the description of spin-dependent interactions in quite generic terms and for the design of experiments in the emergent field of superconducting spintronics.

Candidates should be motivated students with a good background in quantum mechanics and statistical physics, communication skills and good English knowledge. The PhD student will have a unique chance to interact with two renowned groups with a vast experience on mesoscopic superconductivity and magnetism.
More details:
Mesoscopic physics at CFM – San-Sebastián:
http://cfm.ehu.es/mesoscopics/
Exotic Correlated Quantum States at LOMA – Bordeaux:
https://www.loma.cnrs.fr/equipe-exostates/
https://en.wikipedia.org/wiki/Alexandre_Bouzdine

PROJECT 3.- Quantum transport in hybrid structure with semimetals, excitonic insulators and superconductors.

Contact persons: Dario Bercioux (DIPC, dario.bercioux@dipc.org) and Jérôme Cayssol (U. Bordeaux, jerome.cayssol@u-bordeaux.fr)

We are looking for a PhD student to work on a cooperative project between the Mesoscopic Physics Group at the DIPC (Dr. Dario Bercioux) and the Condensed matter theory group at LOMA University of Bordeaux (Prof. Jérôme Cayssol).

The PhD student will be offered different topics in the field of quantum transport in exotic hybrid structures with superconductors, semi-metals and excitonic insulators. During the PhD, the candidate will be introduced to the Landauer-Büttiker formalisms for quantum transport, to non-equilibrium Green function technique and to the fundamental knowledge of superconductivity (BCS theory, Bogoliubov de Gennes equations, Gorkov and quasiclassical Green functions). Within this project, the transport properties of single or multiple interfaces among superconductors, semi-metals and excitonic insulators will be investigated. We will also investigate the effect of a periodic external driving on such exotic phases using the Floquet formalism. Time-dependent driving (from GHz to optical frequency) produce non-equilibrium populations of charge carriers and change the topological character of the bands.

Excitonic insulators were predicted long ago, they are condensate phase of matter similar to superconductivity. However the condensate is constitute by electron-hole pairs instead of Cooper pairs. So far, it has been an elusive phase in solid state systems. Some recent experimental result hints the possibility to have such a phase in HgTe quantum wells. The goal of this project to find smoking gun signature of this phase by combining its condensate properties with the traditional one of superconductors.

Candidates should be motivated students with a good background in quantum mechanics and statistical physics, communication skills and good English knowledge. The PhD student will have a unique chance to interact with two renowned groups with a vast experience on mesoscopic superconductivity and quantum transport.

More details:
Mesoscopic physics at DIPC/CFM – San-Sebastián:
http://www.dario-bercioux.eu/
http://cfm.ehu.es/mesoscopics/
Exotic Correlated Quantum States at LOMA – Bordeaux:
https://www.loma.cnrs.fr/equipe-exostates/
https://www.loma.cnrs.fr/jerome-cayssol/