CURRÍCULUM VÍTAE NORMALIZADO

Pedro Brandimarte Mendonca

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GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN

FECYT FUNDACIÓN ESPAÑOLA PARA LA CIENCIA Y LA TECNOLOGÍA

Summary of CV

This section describes briefly a summary of your career in science, academic and research; the main scientific and technological achievements and goals in your line of research in the medium -and long- term. It also includes other important aspects or peculiarities.

With a background in computational and theoretical physics, and mathematics, he has been working mostly on theoretical modeling and on the development of numerical methods for multi scale simulations. Carries extensive experience on scientific software development, with a deep knowledge on algorithms, abstract data structures, hybrid parallel programming and high-performance computing.

Since the Ph.D. in 2014, he's been working on the development and application of computational tools to model electronic structure and quantum transport at the nanoscale. His research as a graduate student focused on the role of electron-phonon interactions in first principles transport simulations. Among other tools, he developed the program Inelastic DISORDER, which allows one to compute the elastic and inelastic transport properties for large realistic systems (~10.000 atoms) with randomly positioned defects.

He has done postdoctoral stays at the Centro de Física de Materiales and at the Donostia International Physics Center. His research has mainly been devoted to the electronic structure characterization and transport analysis of low-dimensional systems (1D and 2D), such as doped graphene nanoribbons, semiconducting surfaces and multi-terminal devices. In general, his work can be characterized as different successful contributions towards realistic simulations of electronic devices through the development and the application of the state-of-the-art tools. One emblematic example is the first realization of self-consistent calculations of multi-terminal devices via first principles and under non-equilibrium conditions, done with two crossing graphene nanoribbons which revealed a 50/50 beam splitter effect for electrons when the crossing happens at 60 degrees (**JCP 2017**). Another quantum optic analogue for electrons was discovered at the same year on graphene nanoribbons doped with boron moieties, namely an electron equivalent to a Fabry-Perot resonator (**Nano Lett. 2017** and **JPCC 2018**). Using the same kind of nanoribbons, but attaching nitrile functional groups at the edges, revealed a very effective n-doping effect whose mechanism was elucidated via first-principles simulations (**ACS Nano 2017**). The multi-terminal methodology has also been applied very recently to the study of surface transport via a two-probe STM setup (**Nat. Comm. 2019**, with statement of equally contribution as the first experimental author). Another work of him is the implementation of a new methodology for performing molecular dynamics in systems under bias, which is particularly interesting for the simulation of electrochemical cells (**Chem. Sci. 2018**). Recently, the developed knowledge on the field was used to give significant contributions on the magnetism of topological states (**ACS Nano 2019** and **PRL 2020**).

He's joined Alerion Technologies in 2020, where he is contributing in tasks related to computer vision, parallel imaging processing in embedded GPU, autonomous localization and mapping.

General quality indicators of scientific research

This section describes briefly the main quality indicators of scientific production (periods of research activity, experience in supervising doctoral theses, total citations, articles in journals of the first quartile, H index...). It also includes other important aspects or peculiarities.

Author of 16 publications, **10 as first theory author**, in high-quality peer-reviewed journals such as Nature Communications, ACS Nano, Physical Review Letters and Nano Letters, with an **averaged impact factor of 8.64** and **all publications in Q1**.

Pedro Brandimarte Mendonca

Surname(s): **Brandimarte Mendonca**
Name: **Pedro**
ORCID: **0000-0002-8762-5876**
ResearcherID: **G-1307-2016**
Contact aut. region/reg.: **Basque Country**
Personal web page: **https://brandimarte.github.io**

Current professional situation

Employing entity: Alerion Technologies **Type of entity:** Business
Professional category: Software Engineer
Start date: 01/07/2020
Type of contract: Permanent employment contract **Dedication regime:** Full time
Primary (UNESCO code): 220300 - Electronícs; 221100 - Solid state physics; 221200 - Theoretical physics
Secondary (UNESCO code): 221110 - Electron states; 221111 - Electron transport properties; 221125 - Semiconductors
Performed tasks: Computer vision, parallel imaging processing in embedded GPU, autonomous localization and mapping.
Identify key words: Fisica lm -- sistemas de bajas dimensiones y mesoscopicos [eng]; Physics - Semiconductors and band structure

Previous positions and activities

	Employing entity	Professional category	Start date
1	Donostia International Physics Center	Postdoctoral researcher	01/10/2017
2	CENTRO DE FISICA DE MATERIALES	Posdoctoral researcher	28/04/2015
3	European Organization for Nuclear Research - CERN	Scientific Training	01/08/2006
4	University of São Paulo	Scientific Training	01/08/2004

1 **Employing entity:** Donostia International Physics Center
Professional category: Postdoctoral researcher
Start-End date: 01/10/2017 - 30/06/2020 **Duration:** 2 years - 8 months
Type of contract: Temporary employment contract
Performed tasks: Theoretical investigation of functional graphene-based nanostructures and networks for electronics and electron quantum optics applications, such as electronic beam splitters and quantum dots, and of their potential for quantum information processing tasks.

2 **Employing entity:** CENTRO DE FISICA DE MATERIALES **Type of entity:** State agency
City employing entity: San Sebastián - Donostia, Basque Country, Spain

Professional category: Posdoctoral researcher
Start-End date: 28/04/2015 - 30/09/2017 **Duration:** 2 years - 5 months - 2 days
Type of contract: Grant-assisted student (pre or post-doctoral, others)
Dedication regime: Full time
Primary (UNESCO code): 220300 - Electronícs; 221100 - Solid state physics; 221200 - Theoretical physics
Secondary (UNESCO code): 221110 - Electron states; 221111 - Electron transport properties; 221125 - Semiconductors
Performed tasks: Development of tools and theoretical models for studying electron transport in planar atomic and molecular scale devices. Funding: European Commission, 7o Framework Programme (Planar atomic and molecular scale devices - PAMS, C-ICT/3280, ICT Collaborative project, contract 610446).
Identify key words: Physics - Atomic and molecular physics; Fisica lm -- sistemas de bajas dimensiones y mesoscopicos [eng]; Physics - Semiconductors and band structure; Physics - Quantum physics

3 **Employing entity:** European Organization for Nuclear Research - CERN **Type of entity:** R&D Centre
City employing entity: Geneva, Switzerland
Professional category: Scientific Training
Start-End date: 01/08/2006 - 31/01/2007 **Duration:** 6 months
Type of contract: Grant-assisted student (pre or post-doctoral, others)
Dedication regime: Full time
Primary (UNESCO code): 120326 - Simulation; 221200 - Theoretical physics; 229001 - Theoretical Physics high-energy
Performed tasks: Development on the AliRoot framework for simulation at the ALICE Off-line group. Grant: HELEN program (High Energy Latin American Network).
Identify key words: Software; Physics - High energies - Phenomenology; Physics - High energies -

4 **Employing entity:** University of São Paulo
Department: Physics Institute
City employing entity: São Paulo, Brazil
Professional category: Scientific Training
Start-End date: 01/08/2004 - 31/07/2005 **Duration:** 1 year
Type of contract: Grant-assisted student (pre or post-doctoral, others)
Primary (UNESCO code): 220900 - Optics
Secondary (UNESCO code): 220900 - Optics
Performed tasks: Development of a magneto-optical trap (MOT) experiment under the supervision of Prof. Paulo A. Nussenzveig. Grant: National Council of Technological and Scientific Development (CNPq) / Institutional Scholarship Program for Scientific Initiation (PIBIC) - 112144/2004-7.
Identify key words: Physics - Atomic and molecular physics; Physics - Quantum and nonlinear optics; Physics - Optical physics; Physics - Quantum physics

Education

University education

1st and 2nd cycle studies and pre-Bologna degrees

University degree: Higher degree
Name of qualification: Bachelor in Physics
City degree awarding entity: São Paulo, Brazil
Degree awarding entity: University of São Paulo **Type of entity:** University
Date of qualification: 31/07/2007
Standardised degree: No
Foreign qualification: Bacharel em Física (grado en Fisica)

Doctorates

Doctorate programme: Doctor in Science (Physics)
Degree awarding entity: University of São Paulo **Type of entity:** University
City degree awarding entity: São Paulo, Brazil
Date of degree: 03/10/2014
Thesis title: Study of the Influence of Localized Vibrational Modes in Charge Transport Properties at Nanoscale Systems
Thesis director: Antônio José Roque da Silva
Thesis co-director: Alexandre Reily Rocha
Standardised degree: Yes **Date of standardisation:** 11/03/2015

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
French	B2	B1	B1	B1	B1
Spanish	C1	C1	B2	B2	B2
English	C1	C1	C1	C1	C1
Portuguese	C2	C2	C2	C2	C2

Teaching experience

General teaching experience

1 **Name of the course:** Experimental Physics IV
University degree: Bachelor
Start date: 01/02/2005 **End date:** 01/07/2005
Entity: São Paulo University **Type of entity:** University
Faculty, institute or centre: Physics Institute
City of entity: São Paulo, Brazil

2 **Name of the course:** Experimental Physics III
University degree: Bachelor
Start date: 01/07/2004 **End date:** 01/12/2004
Entity: São Paulo University **Type of entity:** University
Faculty, institute or centre: Physics Institute
City of entity: São Paulo, Brazil

Experience supervising doctoral thesis and/or final year projects

1 **Project title:** Electronic properties and tight-binding parametrization of twisted bi-layer graphene.
Type of project: Summer Internship
Co-director of thesis: Pedro Brandimarte; Thomas Frederiksen
Entity: University College London, Faculty of Maths and Physical Sciences **Type of entity:** University
Student: Itsaso Blanco Gonzalez
Date of reading: 10/06/2019

2 **Project title:** Simulations of wave package dynamics in graphene-based materials.
Type of project: Summer Internship
Co-director of thesis: Thomas Frederiksen; Pedro Brandimarte
Entity: Universidad del País Vasco, Departamento de Física
Student: Asier Rodríguez
Date of reading: 10/06/2019

3 **Project title:** Bond order of graphene-based nanostructures
Type of project: Summer Internship
Co-director of thesis: Pedro Brandimarte; Thomas Frederiksen
Entity: Universidad del País Vasco, Departamento de Matemáticas **Type of entity:** University
Student: Amaia Juaristi Arrizabalaga
Date of reading: 21/08/2018

4 **Project title:** Quantum transport in nanoscale devices
Type of project: Summer Internship
Co-director of thesis: Thomas Frederiksen; Pedro Brandimarte
Entity: Universitat de Barcelona, Facultat de Química **Type of entity:** University
Student: Biel Martinez Diaz
Date of reading: 21/08/2018

Educational or pedagogical publications, books, articles, etc.

Zwinglio O. Guimarães-Filho; Leandro Mariano; Pedro Brandimarte; Aline Regis Faro; Ricardo B. Malaquias. Learning physics with high precision experiments at didactic lab: the study of a falling body, Anais do XVI snef 2005. (Brazil): 24/01/2005. Available on-line at: <http://www.sbf1.sbfisica.org.br/eventos/snef/xvi/cd/resumos/t0291-3.pdf>. ISBN 85-89064-08-5
Name of the materials: Article on teaching
Date of drafting: 24/01/2005
Format: Article(s)
Degree of contribution: Author or co-author of educational publication
Position of signature: 3

Participation in conferences with talks focused on teacher training

Name of the event: XVI Simpósio Nacional de Ensino de Física (snef)
Type of event: Conference
Type of participation: Participatory - oral communication
Presentation language: Portuguese
City of event: Rio de Janeiro, Brazil
Date of presentation: 25/01/2005
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Learning physics with high precision experiments at didactic lab: the study of a falling body (Aprendendo física com o uso de experimentos de grande precisão em laboratórios didáticos: o estudo da queda de um corpo). Available on-line at: <http://www.sbf1.sbfisica.org.br/eventos/snef/xvi/programa/mostraresumo.asp?insId=291&traId=3>.

Scientific and technological experience

Scientific or technological activities

R&D projects funded through competitive calls of public or private entities

1 **Name of the project:** GRANAS - A Novel Platform for Electronics and Quantum Electron Optics Based on Graphene Nanostructures
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Donostia International Physics Center **Type of entity:** Research Institute
City of entity: Donostia - San Sebastián, Basque Country, Spain
Name principal investigator (PI, Co-PI....): Thomas Frederiksen; Geza Giedke
Nº of researchers: 3
Funding entity or bodies:
Spanish Ministry of Economy, Industry and Competitiveness **Type of entity:** Public Research Body
City funding entity: Madrid, Community of Madrid, Spain

Type of participation: Team member
Name of the programme: Programa Estatal de Fomento de la Investigación, Científica y Técnica de Excelencia, Subprograma Estatal de Generación de Conocimiento
Code according to the funding entity: FIS2017-83780-P
Start-End date: 01/01/2017 - 01/01/2020 **Duration:** 3 years

2 **Name of the project:** FUNMOLDEV - Theory of Functional Molecular Nanostructures for Optoelectronic Devices
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Name principal investigator (PI, Co-PI....): Daniel Sánchez-Portal
Funding entity or bodies:
Spanish Ministry of Economy, Industry and Competitiveness
City funding entity: Madrid, Community of Madrid, Spain

Type of participation: Team member
Code according to the funding entity: MAT2016-78293-C6-4-R
Start-End date: 2017 - 2019 **Duration:** 2 years

3 **Name of the project:** PAMS - Planar Atomic and Molecular Scale devices (FP7 FET-ICT)
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** European Union
Degree of contribution: Researcher
Name principal investigator (PI, Co-PI....): Daniel Sánchez-Portal
Funding entity or bodies:
European Commission

Type of participation: Team member
Name of the programme: 7th Framework Programme (FP7) on Future and Emerging Technologies (FET) - ICT
Code according to the funding entity: 610446
Start-End date: 01/10/2013 - 30/09/2017 **Duration:** 4 years

4 **Name of the project:** SUPERHYBRID - Theory of Electronic Properties of Covalent Hybrids on Surfaces
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Name principal investigator (PI, Co-PI....): Daniel Sánchez-Portal
Funding entity or bodies:
Spanish Ministry of Economy, Industry and Competitiveness
City funding entity: Madrid, Community of Madrid, Spain

Type of participation: Team member
Code according to the funding entity: MAT2013-46593-C6-2-P
Start-End date: 2014 - 2016 **Duration:** 2 years

Scientific and technological activities

Scientific production

H index: 11
Date of application: 07/02/2021
Fuente de Indice H: GOOGLE SCHOLAR

Publications, scientific and technical documents

1 Jingcheng Li; Pedro Brandimarte; Manuel Vilas-Varela; Nestor Merino-Díez; Cesar Moreno; Aitor Mugarza; Jaime Sáez Mollejo; Daniel Sánchez-Portal; Dimas Garcia de Oteyza; Martina Corso; Aran Garcia-Lekue; Diego Peña; Jose Ignacio Pascual. Band Depopulation of Graphene Nanoribbons Induced by Chemical Gating with Amino Groups. ACS Nano. 14 - 2, pp. 1895 - 1901. American Chemical Society (ACS), 2020.

Type of production: Scientific paper
Format: Journal
Position of signature: 2
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 13
Corresponding author: No
Impact source: ISI
Impact index in year of publication: 14.588

Relevant results: My role in this work was to carry out the electronic structure calculations and analysis of the electrostatics upon chemical doping, which were fundamental for the interpretation of the observed phenomena. We reported on the on surface synthesis of chiral graphene nanoribbons with amino functional groups attached at the edges which lead to an upshift of the bands.
Relevant publication: Yes

2 Niklas Friedrich; Pedro Brandimarte; Jingcheng Li; Shohei Saito; Shigehiro Yamaguchi; Iago Pozo; Diego Peña; Thomas Frederiksen; Aran Garcia-Lekue; Daniel Sánchez-Portal; José Ignacio Pascual. Magnetism of Topological Boundary States Induced by Boron Substitution in Graphene Nanoribbons. Physical Review Letters. 125 - 14, pp. 146801-1 - 146801-6. American Physical Society, 2020.

Type of production: Scientific paper
Format: Journal
Position of signature: 2
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 11
Corresponding author: No
Impact source: ISI
Impact index in year of publication: 9.199

Relevant results: With statement of equally contribution as the first experimental author, in this work I've carried out all the simulations and contributed on the interpretation of the observed phenomena. The simulations involved gas phase and on metallic substrate calculations of graphene nanoribbons with pairs of substitutional boron atoms inserted in the carbon backbone. Gas phase simulations of a boron-substituted nanoribbons found that boron pairs induce a spin 1 state, while in a configuration suspended between the tip and the sample the calculations revealed that a spin 1/2 state appears upon detachment.
Relevant publication: Yes

3 James Lawrence; Pedro Brandimarte; Alejandro Berdonces-Layunta; Mohammed S. G. Mohammed; Abhishek Grewal; Christopher C. Leon; Daniel Sánchez-Portal; Dimas Garcia de Oteyza. Probing the Magnetism of Topological End-States in 5-Armchair Graphene Nanoribbons. ACS Nano. 14 - 4, pp. 4499 - 4508. American Chemical Society (ACS), 2020.

Type of production: Scientific paper
Format: Journal
Position of signature: 2
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 8
Corresponding author: No
Impact source: ISI
Impact index in year of publication: 14.588

Relevant results: With statement of equally contribution as the first experimental author, in this work I've carried out all the simulations and contributed on the interpretation of a novel observed phenomena. We describe the observation of magnetic states localized at the zigzag termini of narrow 5-armchair graphene nanoribbons, which we demonstrated to be topological in nature.
Relevant publication: Yes

4 Mirco Panighel; Sabela Quiroga; Pedro Brandimarte; Cesar Moreno; Aran Garcia-Lekue; Manuel Vilas-Varela; Dulce Rey; Guillaume Sauthier; Gustavo Ceballos; Diego Peña; Aitor Mugarza. Stabilizing Edge Fluorination in Graphene Nanoribbons. ACS Nano. 14 - 9, pp. 11120 - 11129. American Chemical Society (ACS), 2020.

Type of production: Scientific paper
Format: Journal
Position of signature: 3
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 11
Corresponding author: No
Impact source: ISI
Impact index in year of publication: 14.588

Relevant results: In this work I've carried out all the simulations, which comprises not only gas phase calculation, but also on substrate, with a detailed analysis of the electronic structure and dissociation energies. In the work we report the synthesis of edge fluorination in graphene nanoribbons by carefully design of precursors.
Relevant publication: Yes

5 Marek Kolmer; Pedro Brandimarte; Jakub Lis; Rafal Zuzak; Szymon Godlewski; Hiroyo Kawai; Aran Garcia-Lekue; Nicolas Lorente; Thomas Frederiksen; Christian Joachim; Daniel Sánchez-Portal; Marek Szymonski. Electronic transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy. Nature Communications. Springer Nature, 2019.

Type of production: Scientific paper
Format: Journal
Position of signature: 2
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 12
Impact source: ISI
Impact index in year of publication: 12.353

Relevant results: With statement of equally contribution as the first experimental author, in this work I've carried out all the simulations and contributed on the interpretation of a novel and complex experimental setup. We demonstrate quasi-one-dimensional electronic transport along the dimer rows on a Germanium surface using an atomically precise two probe scanning tunneling microscopy protocol and state-of-the-art multi-terminal first-principles transport calculations. We performed a extensive study of the Ge surface states, starting from detailed electronic structure calculations, transport eigenchannels on a Ge surface containing a monoatomic step edge, until realistic transport simulations with single and two STM tips addressing the surface. The simulated systems involved up to five thousand atoms and four terminals (two for the metallic tips and other two for the semiconducting Ge surface), and required us to develop a new methodology for the energy alignment of the different parts of the simulations.
Relevant publication: Yes

6 Luana Sucupira Pedroza; Pedro Brandimarte; Alexandre Reily Rocha; Marivi V. Fernández-Serra. Bias-dependent local structure of water molecules at a metallic interface. Chemical Science. 9 - 1, pp. 62 - 69. Royal Society of Chemistry (RSC), 2018. Available on-line at: <http://pubs.rsc.org/en/Content/ArticleLanding/2018/SC/C7SC02208E>. ISSN 2041-6520

DOI: 10.1039/c7sc02208e
Type of production: Scientific paper
Format: Journal
Position of signature: 2
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 4

Impact source: ISI
Impact index in year of publication: 9.063

Source of citations: WOS
Citations: 3

Relevant results: My main contribution in this work was the implementation on the SMEAGOL code of the forces calculation in a non-equilibrium situation, which allows to perform molecular dynamics together with electronic transport with an applied bias voltage. I also contributed on analyzing all the results, interpreting them and writing the paper. We report the application of this new methodology on the study of the electronic properties and atomic forces of water at the interfaces of metallic electrodes, which allowed us to accurately simulate how the water molecules rearrange under an applied external potential via first principles methods. We find that the water molecule tends to align its dipole moment with the electric field, and it is either repelled or attracted to the metal depending on the sign and magnitude of the applied bias, in an asymmetric fashion.
Relevant publication: Yes

7 Rafal Zuzak; Jesus Castro; Pedro Brandimarte; Mads Engelund; Agustín Cobas; Piotr Piatkowski; Marek Kolmer; Dolores Pérez; Enrique Guitián; Marek Szymonski; Daniel Sánchez-Portal; Szymon Godlewski; Diego Peña. Building a 22-ring nanographene by combining in-solution and on-surface synthesis. Chemical Communications. 54 - 73, pp. 10256 - 10259. Royal Society of Chemistry (RSC), 2018. Available on-line at: <https://pubs.rsc.org/en/Content/ArticleLanding/2018/CC/C8CC05353G>. ISSN 1359-7345
DOI: 10.1039/c8cc05353g
Type of production: Scientific paper
Format: Journal
Position of signature: 3
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 13

Impact source: ISI
Impact index in year of publication: 6.290

Source of citations: WOS
Citations: 1

Relevant results: My role in this work was to carry out the electronic structure calculations, interpret the results and write the theoretical part of the paper. We report on the synthesis of a three-fold symmetric nanographene formed by the fusion of 22 benzene rings prepared by combining in-solution Pd-catalyzed cycloaddition reaction and on-surface Au-promoted cyclodehydrogenation. The structure and electronic properties of the resulting molecule were characterized by scanning probe microscopy with atomic resolution and by the theoretical modelling.
Relevant publication: Yes

8 Eduard Carbonell-Sanromà; Aran Garcia-Lekue; Martina Corso; Guillaume Vasseur; Pedro Brandimarte; Jorge Lobo-Checa; Dimas G. de Oteyza; Jingcheng Li; Shigeki Kawai; Shohei Saito; Shigehiro Yamaguchi; Jose Enrique Ortega; Daniel Sánchez-Portal; Jose Ignacio Pascual. Electronic Properties of Substitutionally Boron-Doped Graphene Nanoribbons on a Au(111) Surface. The Journal of Physical Chemistry C. 122 - 28, pp. 16092 - 16099. American Chemical Society (ACS), 2018. Available on-line at: <https://pubs.acs.org/doi/10.1021/acs.jpcc.8b03748>. ISSN 1932-7447
DOI: 10.1021/acs.jpcc.8b03748
Type of production: Scientific paper
Format: Journal
Position of signature: 5
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 14

Impact source: ISI

Impact index in year of publication: 4.484

Relevant results: My contribution in this work was to perform all gas phase calculations, analyze and interpret the results, as well as helping on writing the theoretical parts of the paper. We describe a detailed study of the electronic structure of GNRs substitutionally doped with di-boron moieties at the center, through a combination of scanning tunneling spectroscopy, angle-resolved photoemission, and density functional theory simulations. We demonstrated that due to the selective mixing of boron states with GNR bands according to their symmetry, the boron atoms causes the shift of the conduction and valence bands of the pristine GNR away from the gap edge, and leave unaffected the bands above and below, which become the new frontier bands and have negligible boron character.

Relevant publication: Yes

9 Pedro Brandimarte; Mads Engelund; Nick Papior; Aran Garcia-Lekue; Thomas Frederiksen; Daniel Sánchez-Portal. A tunable electronic beam splitter realized with crossed graphene nanoribbons. The Journal of Chemical Physics. 146 - 9, pp. 092318. American Institute of Physics (AIP) Publishing, 2017. Available on-line at: <http://aip.scitation.org/doi/full/10.1063/1.4974895>. ISSN 0021-9606

DOI: 10.1063/1.4974895

Type of production: Scientific paper

Format: Journal

Position of signature: 1

Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 6

Impact source: ISI

Impact index in year of publication: 2.843

Source of citations: WOS

Citations: 5

Relevant results: My role in this work was to perform all the calculations, analyze the data and write the paper. This was the first application of the multi-terminal implementation on the TranSIESTA code. We explore the properties of a prototype 4-terminal semiconducting device formed by two crossed armchair GNRs using state-of-the-art first-principles transport methods. We analyze in detail the roles of intersection angle, stacking order, inter-GNR separation, GNR width, and finite voltages on the transport characteristics. We showed that at an intersection angle of 60 degrees the two AGNRs crossing can operate as an electronic beam splitter where the ratio of intra/inter transmission can be tuned by changing the inter-GNR distance, i.e., it can be mechanically controlled by applying an external force to the junction.

Relevant publication: Yes

10 Eduard Carbonell-Sanromà; Jeremy Hieulle; Manuel Vilas-Varela; Pedro Brandimarte; Mikel Iraola; Ana Barragán; Jingcheng Li; Mikel Abadia; Martina Corso; Daniel Sánchez-Portal; Diego Peña; Jose Ignacio Pascual. Doping of Graphene Nanoribbons via Functional Group Edge Modification. ACS Nano. 11 - 7, pp. 7355 - 7361. American Chemical Society (ACS), 2017. Available on-line at: <http://pubs.acs.org/doi/abs/10.1021/acsnano.7b03522>. ISSN 1936-0851

DOI: 10.1021/acsnano.7b03522

Type of production: Scientific paper

Format: Journal

Position of signature: 4

Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 12

Impact source: ISI

Impact index in year of publication: 13.709

Citations: 19

Relevant results: My role in this work was to perform all the calculations, analyze and interpret, and write the theoretical part of the paper. We report the on-surface synthesis of 7-armchair graphene nanoribbons substituted with nitrile functional groups, which are attached to the GNR edge. Scanning tunneling spectroscopy and density functional theory reveal that CN groups behave as very efficient n-dopants, significantly downshifting the bands of the ribbon and introducing deep impurity levels associated with the nitrogen electron lone pairs.

Relevant publication: Yes

11 Eduard Carbonell-Sanromà; Pedro Brandimarte; Richard Balog; Martina Corso; Shigeki Kawai; Aran Garcia-Lekue; Shohei Saito; Shigehiro Yamaguchi; Ernst Meyer; Daniel Sánchez-Portal; Jose Ignacio Pascual. Quantum Dots Embedded in Graphene Nanoribbons by Chemical Substitution. Nano Letters. 17 - 1, pp. 50 - 56. American Chemical Society (ACS), 2017. Available on-line at: <http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.6b03148>. ISSN 1530-6984

DOI: 10.1021/acs.nanolett.6b03148

Type of production: Scientific paper

Position of signature: 2

Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 11

Impact source: ISI

Impact index in year of publication: 12.080

Source of citations: WOS

Citations: 20

Relevant results: My role in the work was to perform all the calculations, which required the implementation on the SIESTA code of an exact Coulomb cutoff method for low dimension systems. I've analyzed and interpreted the results, and wrote the theoretical part of the paper. We report on the formation of quantum dots embedded in an armchair GNR by substitutional inclusion of pairs of boron atoms into the GNR backbone. In the pristine region between two boron pairs, the nanoribbons show a discretization of their valence band into confined modes compatible with a Fabry-Perot resonator. Electronic structure and transport simulations reveal that they selectively confine the first valence band of the pristine ribbon while allowing an efficient electron transmission of the second one.

Relevant publication: Yes

12 Mads Engelund; Nick Papior; Pedro Brandimarte Mendonca; Thomas Frederiksen; Aran Garcia-Lekue; Daniel Sáchez-Portal. Search for a Metallic Dangling-Bond Wire on n-Doped H-Passivated Semiconductor Surfaces. Journal of Physical Chemistry C. 120 - 36, pp. 20303 - 20309. American Chemical Society (ACS), 2016. Available on-line at: <http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b04540>. ISSN 1932-7447

DOI: 10.1021/acs.jpcc.6b04540

Type of production: Scientific paper

Format: Journal

Position of signature: 3

Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 5

Impact source: ISI

Impact index in year of publication: 4.5360

Source of citations: WOS

Citations: 6

Relevant results: My main contribution to this work was the implementation on the SIESTA code of spin contamination analysis, which was used to determine the amount of spin contamination in the studied systems. We investigate the electronic and transport properties of neutral and n-doped dangling bond quasi-one-dimensional structures in the Si(001):H and Ge(001):H substrates with the aim of identifying atomic-scale interconnects exhibiting metallic conduction for use in on-surface circuitry.

Relevant publication: Yes

13 Cesar E. P. Villegas; Pedro Brandimarte Mendonca; Alexandre Reily Rocha. Optical spectrum of bottom-up graphene nanoribbons: Towards efficient atom-thick excitonic solar cells. Scientific Reports. 4 - 1, pp. 6579. Springer Nature, 2014. Available on-line at: <http://www.nature.com/srep/2014/141010/srep06579/full/srep06579.html>. ISSN 2045-2322

DOI: 10.1038/srep06579

Type of production: Scientific paper

Format: Journal

Position of signature: 2

Degree of contribution: Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 3

Impact source: ISI

Impact index in year of publication: 5.578

Source of citations: WOS **Citations:** 12

Relevant results: In this work I've contributed with all the electronic structure and transport calculations, as well as with the interpretation of the results. We carry out ab-initio density functional theory calculations combined with many-body perturbation formalism to study the electronic and optical properties of atomically well-defined cove-shaped graphene nanoribbons that were previously synthesized. We found that the excitonic peaks in the absorption spectrum are a consequence of a group of transitions involving the first and second conduction and valence bands, in contrast to zigzag graphene nanoribbons. We also estimate some relevant optical properties that strengthen the potential of these nanoribbons for acting as a donor materials in photovoltaic.

Relevant publication: Yes

14 Sofia Sanz; Pedro Brandimarte; Géza Giedke; Daniel Sánchez-Portal; Thomas Frederiksen. Crossed graphene nanoribbons as beam splitters and mirrors for electron quantum optics. Physical Review B. 102 - 3, pp. 035436-1 - 035436-14. American Physical Society (APS), 2020.

Type of production: Scientific paper **Format:** Journal

Position of signature: 2 **Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 5 **Corresponding author:** No

Impact source: ISI

Impact index in year of publication: 3.721

Relevant results: In this theoretical work we provide a detailed description of four-terminal devices composed by crossing two graphene nanorribons, considering different edge topologies, stackings, intersection angle etc, highlighting the potential candidates for electronic beam splitters and for mirrors.

15 Rafal Zuzak; Pedro Brandimarte; Piotr Olszowski; Irena Izydorczyk; Marios Markoulides; Bartosz Such; Marek Kolmer; Marek Szymonski; Aran Garcia-Lekue; Daniel Sánchez-Portal; André Gourdon; Szymon Godlewski. On-Surface Synthesis of Chlorinated Narrow Graphene Nanoribbon Organometallic Hybrids. Journal of Physical Chemistry Letters. 11 - 24, pp. 10290 - 10297. American Chemical Society (ACS), 2020.

Type of production: Scientific paper **Format:** Journal

Position of signature: 2 **Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 12 **Corresponding author:** No

Impact source: ISI

Impact index in year of publication: 6.71

Relevant results: In this work I've performed all the simulations and theoretical analysis, which involved both gas phase and on substrate density functional theory calculations.

16 Alberto García; Nick Papior; Arsalan Akhtar; Emilio Artacho; Volker Blum; Emanuele Bosoni; Pedro Brandimarte; Mads Brandbyge; J. I. Cerdá; Fabiano Corsetti; Ramón Cuadrado; Vladimir Dikan; Jaime Ferrer; Julian Gale; Pablo García-Fernández; V. M. García-Suárez; Sandra García; Georg Huhs; Sergio Illera; Richard Korytár; Peter Koval; Irina Lebedeva; Lin Lin; Pablo López-Tarifa; Sara G. Mayo; Stephan Mohr; Pablo Ordejón; Andrei Postnikov; Yann Pouillon; Miguel Pruneda; Roberto Robles; Daniel Sánchez-Portal; Jose M. Soler; Rafi Ullah; Victor Wen-zhe Yu; Javier Junquera. Siesta: Recent developments and applications. Journal of Chemical Physics. 152 - 20, pp. 204108-1 - 204108-31. AIP Publishing, 2020.

Type of production: Scientific paper **Format:** Journal

Position of signature: 7 **Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee

Total no. authors: 36 **Corresponding author:** No

Impact source: ISI

Impact index in year of publication: 2.974

Relevant results: My contribution in this work was the description of large scale multi-terminal simulation systems composed by both metallic and semiconducting electrodes.

Works submitted to national or international conferences

1 **Title of the work:** Emerging magnetism in boron-doped graphene nanoribbons
Name of the conference: 3S'20 - Symposium on Surface Science 2020
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: St.Christoph/Arlberg, Austria
Date of event: 01/03/2020
End date: 07/03/2020
Organising entity: TU Wien - Institut für Angewandte Physik **Type of entity:** University
Pedro Brandimarte; Niklas Friedrich; Jingcheng Li; Shohei Saito; Shigehiro Yamaguchi; Iago Pozo; Diego Peña; Thomas Frederiksen; Aran Garcia-Lekue; Daniel Sánchez-Portal; José Ignacio Pascual. Available on-line at: <https://www.iap.tuwien.ac.at/www/3s20/index>.

2 **Title of the work:** Probing the magnetism of topological end-states in 5-armchair graphene nanoribbons
Name of the conference: 3S'20 - Symposium on Surface Science 2020
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: St.Christoph/Arlberg, Austria
Date of event: 01/03/2020
End date: 07/03/2020
Organising entity: TU Wien - Institut für Angewandte Physik **Type of entity:** University
James Lawrence; Pedro Brandimarte; Alejandro Berdonces-Layunta; Mohammed S. G. Mohammed; Abhishek Grewal; Christopher C. Leon; Daniel Sánchez-Portal; Dimas G. de Oteyza. Available on-line at: <https://www.iap.tuwien.ac.at/www/3s20/index>.

3 **Title of the work:** DFT exploration of magnetic properties in substitutionally doped graphene nanoribbons
Name of the conference: Computational Physics and Materials Science: Total Energy and Force Methods
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 08/01/2020
End date: 10/01/2020
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
Rodrigo Menchon; Pedro Brandimarte; Daniel Sánchez-Portal; Aran Garcia-Lekue. Available on-line at: <http://totalenergy2020.dipc.org/>.

4 **Title of the work:** Deciphering the electronic structure of 5-armchair graphene nanoribbons and its topological end-states
Name of the conference: Computational Physics and Materials Science: Total Energy and Force Methods
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 08/01/2020

End date: 10/01/2020
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
Pedro Brandimarte; James Lawrence; Alejandro Berdonces-Layunta; Mohammed S. G. Mohammed; Dimas G. de Oteyza; Daniel Sánchez-Portal. Available on-line at: <http://totalenergy2020.dipc.org/>.

5 **Title of the work:** Electronic Transport in Mo2ScC2O2 MXene
Name of the conference: Computational Physics and Materials Science: Total Energy and Force Methods
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 08/01/2020
End date: 10/01/2020
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
Emre Bölen; Pedro Brandimarte; Daniel Sánchez-Portal; E. Deligoz. Available on-line at: <http://totalenergy2020.dipc.org/>.

6 **Title of the work:** N-terminal Graphene-based Nanostructures for Electron Quantum Optical setups
Name of the conference: Computational Physics and Materials Science: Total Energy and Force Methods
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 08/01/2020
End date: 10/01/2020
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
Sofia Sanz; Pedro Brandimarte; Daniel Sánchez-Portal; Géza Giedke; Thomas Frederiksen. Available on-line at: <http://totalenergy2020.dipc.org/>.

7 **Title of the work:** Electronic structure of 5-armchair graphene nanoribbons: STM study of their topological end states
Name of the conference: Exploring the Limits of Nanoscience with Scanning Probe Methods
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Bad Honnef, Germany
Date of event: 27/10/2019
End date: 31/10/2019
Organising entity: Wilhelm and Else Heraeus-Foundation
Alejandro Berdonces-Layunta; James Lawrence; Pedro Brandimarte; Mohammed S. G. Mohammed; Daniel Sánchez-Portal; Dimas G. de Oteyza. Available on-line at: <https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2019/exploring-the-limits-of-nanoscience-with-scanning-probe-methods/main/>.

8 **Title of the work:** Electronic structure of 5-armchair graphene nanoribbons: STM study of their topological end states
Name of the conference: Exploring the Limits of Nanoscience with Scanning Probe Methods
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Bad Honnef, Germany
Date of event: 27/10/2019
End date: 31/10/2019
Organising entity: Wilhelm and Else Heraeus-Foundation

Alejandro Berdonces-Layunta; James Lawrence; Pedro Brandimarte; Mohammed S. G. Mohammed; Daniel Sánchez-Portal; Dimas G. de Oteyza. Available on-line at: <https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2019/exploring-the-limits-of-nanoscience-with-scanning-probe-methods/main/>.

9 **Title of the work:** Inducing magnetism in graphene nanoribbons by substitutional Boron-doping
Name of the conference: Exploring the Limits of Nanoscience with Scanning Probe Methods
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Bad Honnef, Germany
Date of event: 27/10/2019
End date: 31/10/2019
Organising entity: Wilhelm and Else Heraeus-Foundation
Niklas Friedrich; Pedro Brandimarte; Jingcheng Li; Iago Pozo; Diego Peña; Thomas Frederiksen; Aran Garcia-Lekue; Daniel Sánchez-Portal; Jose Ignacio Pascual. Available on-line at: <https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2019/exploring-the-limits-of-nanoscience-with-scanning-probe-methods/main/>.

10 **Title of the work:** Inducing magnetism in graphene nanoribbons by substitutional Boron-doping
Name of the conference: N-terminal Graphene-based Nanostructures for Electron Quantum Optical Setups
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Bad Honnef, Germany
Date of event: 27/10/2019
End date: 31/10/2019
Organising entity: Wilhelm and Else Heraeus-Foundation
Sofia Sanz; Pedro Brandimarte; Daniel Sánchez-Portal; Géza Giedke; Thomas Frederiksen. Available on-line at: <https://www.we-heraeus-stiftung.de/veranstaltungen/seminare/2019/exploring-the-limits-of-nanoscience-with-scanning-probe-methods/main/>.

11 **Title of the work:** Multi-probe scanning tunneling spectroscopy for in-plane electronic transport: theory and experiment
Name of the conference: Trends in Nanotechnology International Conference (TNT2019)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 30/09/2019
End date: 04/10/2019
Organising entity: Phantoms Foundation
Pedro Brandimarte; Marek Kolmer; Jakub Lis; Rafal Zuzak; Szymon Godlewski; Hiroyo Kawai; Aran Garcia-Lekue; Nicolas Lorente; Thomas Frederiksen; Christian Joachim; Daniel Sánchez-Portal; Marek Szymonski. Available on-line at: <http://tntconf.archivephantomsnet.net/2019/index.php?conf=19>.

12 **Title of the work:** Realistic multi-terminal fist-principles transport simulations of two-probe STM measurements on Ge(001) surface: demonstration of quasi-ballistic transport through dangling-bond dimer wires
Name of the conference: 3rd Basque Quantum Science and Technology Workshop
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 23/05/2019
End date: 23/05/2019
Type of entity: Research Institute

Organising entity: Donostia International Physics Center

Pedro Brandimarte; Marek Kolmer; Hiroyo Kawai; Thomas Frederiksen; Aran Garcia-Lekue; Nicolas Lorente; Jakub Lis; Rafal Zuzak; Szymon Godlewski; Christian Joachim; Marek Szymonski; Daniel Sánchez-Portal. Available on-line at: <http://dipc.ehu.es/giedke/eusqutech19.html>.

13 **Title of the work:** Transport Experiments Through Individual Graphene Nanoribbons

Name of the conference: DPG Spring Meeting

Type of event: Conference **Geographical area:** Non EU International

Type of participation: 'Participatory - poster

City of event: Regensburg, Germany

Date of event: 31/03/2019

End date: 05/04/2019

Organising entity: Deutsche Physikalische Gesellschaft **Type of entity:** Associations and Groups

City organizing entity: Bad Honnef, Köln, Germany

Niklas Friedrich; Pedro Brandimarte; Jose Ignacio Pascual. Available on-line at: <https://regensburg19.dpg-tagungen.de/index.html?set_language=en&cl=en>.

14 **Title of the work:** Coherent transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy

Name of the conference: Charge Transport with Multi-Tip STM Techniques

Type of event: Workshop **Geographical area:** Non EU International

Type of participation: Participatory - oral communication

City of event: Jülich, Germany

Date of event: 19/09/2018

End date: 21/09/2018

Organising entity: Jülich Forschungszantrum

City organizing entity: Jülich,

M. Kolmer; R. Zuzak; S. Godlewski; M. Szymonski; Pedro Brandimarte; T. Frederiksen; A. Garcia-Lekue; N. Lorente; D. Sánchez-Portal; H. Kawai; C. Joachim. Available on-line at: <https://www.fz-juelich.de/conferences/4pp_workshop2018>.

15 **Title of the work:** Electron beam splitting with crossed graphene nanoribbons

Name of the conference: International conference on Novel 2D materials explored via scanning probe microscopy & spectroscopy

Type of event: Conference **Geographical area:** Non EU International

Type of participation: Participatory - oral communication

City of event: Donostia - San Sebastián, Basque Country, Spain

Date of event: 25/06/2018

End date: 29/06/2018

Organising entity: Donostia International Physics Center **Type of entity:** Research Institute

City organizing entity: Donostia - San Sebastián, Basque Country, Spain

Sofia Sanz; Pedro Brandimarte; Daniel Sánchez-Portal; Geza Giedke; Thomas Frederiksen. En: book of abstracts. Available on-line at: <http://2dspm.dipc.org/images/2DSPM_Book%20Abstracts.pdf>.

16 **Title of the work:** Electronic consequences of chemical doping of 7-Armchair Graphene Nanoribbons

Name of the conference: International conference on Novel 2D materials explored via scanning probe microscopy & spectroscopy

Type of event: Conference **Geographical area:** Non EU International

Type of participation: Participatory - oral communication

City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 25/06/2018
End date: 29/06/2018
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
City organizing entity: Donostia - San Sebastián, Basque Country, Spain
Martina Corso; Eduard Carbonell-Sanromà; Aran Garcia-Lekue; Pedro Brandimarte; Jeremy Hieulle; Manuel Vilas-Varela; Néstor Merino-Díez; Jingcheng Li; Guillaume Vasseur; Jorge Lobo-Checa; Dimas G. de Oteyza; Shigeki Kawai; Mikel Iraola; Ana Barragán; Mikel Abadia; Jose Enrique Ortega; Daniel Sánchez-Portal; Diego Peña; Jose Ignacio Pascual. En: book of abstracts. Available on-line at: <http://2dspm.dipc.org/images/2DSPM_Book%20Abstracts.pdf>.

17 **Title of the work:** Bias-dependent first principles simulations of gold/water interfaces
Name of the conference: Encontro de Outono da Sociedade Brasileira de Física (EOSBF)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Foz do Iguaçu, Brazil
Date of event: 06/05/2018
End date: 11/05/2018
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Luana Sucupira Pedroza; Pedro Brandimarte; Alexandre Reily Rocha; Marivi Fernández-Serra. En: Anais do Encontro de Outono da Sociedade Brasileira de Física 2018. Available on-line at: <http://www1.sbfisica.org.br/eventos/enfmc/xli/sys/resumos/R0273-1.pdf>.

18 **Title of the work:** Realistic multi-terminal first-principles transport simulations of two-probe STM measurements on Ge(001) surface: demonstration of quasi-ballistic transport through dangling-bond dimer wires
Name of the conference: Encontro de Outono da Sociedade Brasileira de Física (EOSBF)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Foz do Iguaçu, Brazil
Date of event: 06/05/2018
End date: 11/05/2018
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Pedro Brandimarte; Marek Kolmer; Hiroyo Kawai; Thomas Frederiksen; Aran Garcia-Lekue; Nicolas Lorente; Rafal Zuzak; Szymon Godlewski; Christian Joachim; Marek Szymonski; Daniel Sánchez-Portal. En: Anais do Encontro de Outono da Sociedade Brasileira de Física 2018. Available on-line at: <http://www1.sbfisica.org.br/eventos/enfmc/xli/sys/resumos/R0634-1.pdf>.

19 **Title of the work:** Quasi-ballistic transport through surface states of Ge(001)-c(4x2) demonstrated by two-probe STM measurements and multi-terminal fist-principles simulations
Name of the conference: DPG Spring Meeting and EPS-CMD27
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Berlin, Berlin, Germany
Date of event: 11/03/2018
End date: 16/03/2018
Organising entity: Deutsche Physikalische Gesellschaft **Type of entity:** Associations and Groups
City organizing entity: Bad Honnef, Köln, Germany

Pedro Brandimarte; Marek Kolmer; Hiroyo Kawai; Thomas Frederiksen; Aran Garcia-Lekue; Nicolas Lorente; Mads Engelund; Rafal Zuzak; Szymon Godlewski; Christian Joachim; Marek Szymonski; Daniel Sánchez-Portal. Available on-line at: <https://www.dpg-verhandlungen.de/year/2018/conference/berlin/part/o/session/29/contribution/6>.

20 **Title of the work:** Tuning the band structures of graphene nanoribbons by functionalized edge groups
Name of the conference: DPG Spring Meeting and EPS-CMD27
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Berlin, Berlin, Germany
Date of event: 11/03/2018
End date: 16/03/2018
Organising entity: Deutsche Physikalische Gesellschaft **Type of entity:** Associations and Groups
City organizing entity: Bad Honnef, Köln, Germany
Jingcheng Li; Néstor Merino-Díez; Eduard Carbonell-Sanromà; Jeremy Hieulle; Manuel Vilas-Varela; Aran Garcia-Lekue; Pedro Brandimarte; Martina Corso; Daniel Sánchez-Portal; Dimas G. de Oteyza; Aitor Mugarza; Diego Peña; Jose Ignacio Pascual. Available on-line at: <https://www.dpg-verhandlungen.de/year/2018/conference/berlin/part/o/session/81/contribution/13>.

21 **Title of the work:** Two-probe STM/STS experiments performed on atomic wires and single molecules supported on Ge(001) surface
Name of the conference: 31 Symposium on Surface Science (3S*18)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: St.Christoph, Austria
Date of event: 25/02/2018
End date: 03/03/2018
Organising entity: Institute of Applied Physics (IAP) - TU Wien
City organizing entity: Vienna, Austria
Marek Kolmer; Pedro Brandimarte; Lukasz Zajac; Rafal Zuzak; Szymon Godlewski; Hiroyo Kawai; Thomas Frederiksen; Mads Engelund; Aran Garcia-Lekue; Nicolas Lorente; Jakub Lis; Antonio M. Echavarren; Christian Joachim; Daniel Sánchez-Portal; Marek Szymonski. En: Book of Abstracts. Available on-line at: <https://www.iap.tuwien.ac.at/www/_media/3s18/book_of_abstracts_3s18.pdf>.

22 **Title of the work:** Towards electronic devices using graphene nanoribbons
Name of the conference: 13th European Conference on Surface Crystallography and Dynamics (ECSCD-13)
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 19/07/2017
End date: 21/07/2017
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
City organizing entity: Donostia - San Sebastián, Basque Country, Spain
Pedro Brandimarte; Mads Engelund; Nick Papior; Aran Garcia-Lekue; Thomas Frederiksen; Daniel Sánchez-Portal. En: Book of Abstracts. Available on-line at: <http://ecscd13.dipc.org/pdfs/BoA_ECSCD13.pdf>.

23 **Title of the work:** 1-D Quantum Well States on Doped Graphene Nanoribbons Revealed by Transport Simulations
Name of the conference: American Physical Society (APS) March Meeting

Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: New Orleans, United States of America
Date of event: 13/03/2017
End date: 17/03/2017
Organising entity: American Physical Society (APS) **Type of entity:** Associations and Groups
City organizing entity: College Park, United States of America
Pedro Brandimarte; Eduard Carbonell-Sanromà; Richard Balog; Martina Corso; Shigeki Kawai; Aran Garcia-Lekue; Shohei Saito; Shigehiro Yamaguchi; Ernst Meyer; Jose Ignacio Pascual; Daniel Sánchez-Portal. En: Proceedings of the 2017 March Meeting of the American Physical Society. Available on-line at: <http://meetings.aps.org/Meeting/MAR17/Session/E31.14>.

24 **Title of the work:** An electronic beam splitter realized with crossed graphene nanoribbons
Name of the conference: American Physical Society (APS) March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: New Orleans, United States of America
Date of event: 13/03/2017
End date: 17/03/2017
Organising entity: American Physical Society (APS) **Type of entity:** Associations and Groups
City organizing entity: College Park, United States of America
Thomas Frederiksen; Pedro Brandimarte; Mads Engelund; Nick Papior; Aran Garcia-Lekue; Daniel Sánchez-Portal. En: Proceedings of the 2017 March Meeting of the American Physical Society. Available on-line at: <http://meetings.aps.org/Meeting/MAR17/Session/A31.8>.

25 **Title of the work:** An electronic beam splitter realized with crossed graphene nanoribbons
Name of the conference: 14th Nanoscience and Nanotechnology (N&N) in Spain Conference
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 07/03/2017
End date: 10/03/2017
Organising entity: Fundación Phantoms **Type of entity:** Foundation
Thomas Frederiksen; Pedro Brandimarte; Mads Engelund; Nick Papior; Aran Garcia-Lekue; Daniel Sánchez-Portal. En: Proceedings of the 14h Nanoscience and Nanotechnology (N&N) in Spain Conference. Available on-line at: <http://www.nanospainconf.org/2017/Abstracts/Nanospain2017_Frederiksen_Thomas_93.pdf>.

26 **Title of the work:** A tunable electronic beam splitter realized with crossed graphene nanoribbons
Name of the conference: 30 Symposium on Surface Science 2017 (3S'17)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: St. Moritz, Switzerland
Date of event: 05/03/2017
End date: 11/03/2017
Organising entity: Empa, Swiss Federal Laboratories for Materials Sciene and Technology **Type of entity:** R&D Centre
City organizing entity: Dübendorf, Switzerland
Pedro Brandimarte; Mads Engelund; Nick Papior; Aran Garcia-Lekue; Thomas Frederiksen; Daniel Sánchez-Portal. En: Proceedings of the Symposium on Surface Science 2017. Available on-line at: <http://3s17.empa.ch/>.

27 **Title of the work:** Band discretization of Armchair Graphene Nanoribbons via chemical modification
Name of the conference: On-Surface Synthesis International Workshop
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 27/07/2016
End date: 30/07/2016
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
City organizing entity: Donostia - San Sebastián, Basque Country, Spain
Eduard Carbonell-Sanromà; Pedro Brandimarte; Martina Corso; Richard Balog; Shigeki Kawai; Aran Garcia-Lekue; Shohei Saito; Shinichiro Osumi; Shigehiro Yamaguchi; Ernst Meyer; Daniel Sánchez-Portal; Jose Ignacio Pascual. En: Proceedings of 2nd On-Surface Synthesis International Workshop. Available on-line at: <http://oss.dipc.org/images/Program_OSS16.pdf>.

28 **Title of the work:** Electronic structure of boron doped graphene nanoribbons
Name of the conference: On-Surface Synthesis International Workshop
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 27/07/2016
End date: 30/07/2016
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
City organizing entity: Donostia - San Sebastián, Basque Country, Spain
Martina Corso; Eduard Carbonell-Sanromà; Guillaume Vasseur; Aran Garcia-Lekue; Pedro Brandimarte; Richard Balog; Shigeki Kawai; Jorge Lobo-Checa; Dimas G. de Oteyza; Enrique Ortega; Daniel Sánchez-Portal; Jose Ignacio Pascual. En: Proceedings of 2nd On-Surface Synthesis International Workshop. Available on-line at: <http://oss.dipc.org/images/Program_OSS16.pdf>.

29 **Title of the work:** Aspects of graphene nanoribbon device simulations
Name of the conference: Towards reality in modelling of molecular electronics (TRMME)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 13/06/2016
End date: 17/06/2016
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
City organizing entity: Donostia - San Sebastián, Basque Country, Spain
Pedro Brandimarte; Nick R. Papior; Mads Engelund; Aran Garcia-Lekue; Thomas Frederiksen; Eduard Carbonell-Sanromà; Martina Corso; Richard Balog; Shigeki Kawai; Shohei Saito; Shinichiro Osumi; Shigehiro Yamaguchi; Jose Ignacio Pascual; Daniel Sánchez-Portal. En: Proceedings of the DIPC-PAMS theory workshop: Towards reality in modelling of molecular electronics (TRMME). Available on-line at: <http://trmme.dipc.org/monday.html#brandimarte>.

30 **Title of the work:** Electron Transport Simulations of 4-Terminal Crossed Graphene Nanoribbons Devices
Name of the conference: American Physical Society (APS) March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Baltimore, United States of America
Date of event: 14/03/2016

End date: 18/03/2016
Organising entity: American Physical Society (APS) **Type of entity:** Associations and Groups
City organizing entity: College Park, United States of America
Pedro Brandimarte; Nick R. Papior; Mads Engelund; Aran Garcia-Lekue; Thomas Frederiksen; Daniel Sánchez-Portal. En: Proceedings of the 2016 March Meeting of the American Physical Society. Available on-line at: <http://meetings.aps.org/Meeting/MAR16/Session/C26.1>.

31 **Title of the work:** First principle simulations of a bias-dependent electrochemical cell
Name of the conference: American Physical Society (APS) March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Baltimore, United States of America
Date of event: 14/03/2016
End date: 18/03/2016
Organising entity: American Physical Society (APS) **Type of entity:** Associations and Groups
City organizing entity: College Park, United States of America
Luana Sucupira Pedroza; Pedro Brandimarte; Marivi Fernandez-Serra; Alexandre R. Rocha. En: Proceedings of the 2016 March Meeting of the American Physical Society. Available on-line at: <http://meetings.aps.org/Meeting/MAR16/Session/H32.11>.

32 **Title of the work:** Electron Transport in Crossed Graphene Nanoribbon Devices: 4-Terminal ab initio Simulations
Name of the conference: CECAM Workshop on 'Open Quantum Systems: Computational Methods'
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Hong Kong, Hong Kong
Date of event: 30/11/2015
End date: 04/12/2015
Organising entity: Centre Européen de Calcul Atomique et Moléculaire (CECAM) **Type of entity:** R&D Centre
City organizing entity: Lausanne, Switzerland
Pedro Brandimarte; Nick R. Papior; Mads Engelund; Aran Garcia-Lekue; Thomas Frederiksen; Daniel Sánchez-Portal. En: Proceedings of the CECAM Workshop on 'Open Quantum Systems: Computational Methods'. Available on-line at: <http:///www.cecam.org/workshop-3-1216.html?poster_id=14942>.

33 **Title of the work:** Inelastic Disordered Transport Applied to Graphene Nanoribbons with Hydroxyl Impurities
Name of the conference: The 15th International Conference on Vibrations at Surfaces
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster
City of event: Donostia - San Sebastián, Basque Country, Spain
Date of event: 22/06/2015
End date: 26/06/2015
Organising entity: Donostia International Physics Center **Type of entity:** Research Institute
City organizing entity: Donostia - San Sebastián, Basque Country, Spain
Pedro Brandimarte; Alberto Torres Riera Junior; Antônio José Roque da Silva; Alexandre Reily Rocha. En: Proceedings of the 15th International Conference on Vibrations at Surfaces. Available on-line at: <http://vas15.dipc.org/abstracts/Mendonca.html>.

34 **Title of the work:** Inelastic Electronic Transport in Disordered Systems
Name of the conference: XXXVIII ENFMC Brazilian Physical Society Meeting 2015
Type of event: Conference **Geographical area:** Non EU International

Type of participation: 'Participatory - poster
City of event: Foz do Iguaçu, Brazil
Date of event: 24/05/2015
End date: 29/05/2015
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Pedro Brandimarte; Alexandre Reily Rocha; Antônio José Roque da Silva. En: Anais do XXXVIII Encontro Nacional de F??sica da Matéria Condensada. Available on-line at: <http://www1.sbfisica.org.br/eventos/enfmc/xxxviii/sys/resumos/R1204-1.pdf>.

35 **Title of the work:** Interaction of water molecules with gold surfaces under the presence of an external potential
Name of the conference: XXXVIII ENFMC Brazilian Physical Society Meeting 2015
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Foz do Iguaçu, Brazil
Date of event: 24/05/2015
End date: 29/05/2015
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Luana Sucupira Pedroza; Pedro Brandimarte; Marivi Fernandez-Serra; Alexandre Reily Rocha. En: Anais do XXXVIII Encontro Nacional de F??sica da Matéria Condensada. Available on-line at: <http://www1.sbfisica.org.br/eventos/enfmc/xxxviii/sys/resumos/R0491-1.pdf>.

36 **Title of the work:** Bias-dependent local structure of water molecules at an electrochemical interface
Name of the conference: American Physical Society (APS) March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: San Antonio, United States of America
Date of event: 02/03/2015
End date: 06/03/2015
Organising entity: American Physical Society (APS) **Type of entity:** Associations and Groups
City organizing entity: College Park, United States of America
Luana Sucupira Pedroza; Pedro Brandimarte; Alexandre R. Rocha; Marivi Fernandez-Serra. En: Proceedings of the 2015 March Meeting of the American Physical Society. Available on-line at: <http://meetings.aps.org/Meeting/MAR15/Session/T34.8>.

37 **Title of the work:** First Principles Analysis Of Metal/water Interaction Under The Influence Of External Bias Potential
Name of the conference: XIII Brazilian MRS (Materials Research Society)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: João Pessoa, Brazil
Date of event: 28/09/2014
End date: 02/10/2014
Organising entity: Brazilian Materials Research Society **Type of entity:** Associations and Groups
City organizing entity: Rio de Janeiro, Brazil
Luana Sucupira Pedroza; Pedro Brandimarte; Alexandre R. Rocha; Marivi Fernandez-Serra. En: Proceedings of the XIII Brazilian MRS Meeting. Available on-line at: <http://sbpmat.org.br/13encontro/?lang=en>.

38 **Title of the work:** First principles molecular dynamics at the electrochemical interface
Name of the conference: XXXVII ENFMC Brazilian Physical Society Meeting 2014
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Costa do Sauípe, Brazil
Date of event: 12/05/2014
End date: 16/05/2014
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Luana Sucupira Pedroza; Pedro Brandimarte; Marivi Fernandez-Serra; Alexandre Reily Rocha. En: Anais do XXXVII Encontro Nacional de F??sica da Matéria Condensada. Available on-line at: <http://www.sbf1.sbfisica.org.br/eventos/enfmc/xxxvii/sys/resumos/R0841-1.pdf>.

39 **Title of the work:** First principles molecular dynamics of metal/water interfaces under bias potential.
Name of the conference: American Physical Society (APS) March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Denver, United States of America
Date of event: 03/03/2014
End date: 07/03/2014
Organising entity: American Physical Society (APS) **Type of entity:** Associations and Groups
City organizing entity: College Park, United States of America
Luana Sucupira Pedroza; Pedro Brandimarte; Alexandre Reyli Rocha; Marivi Fernandez-Serra. En: Proceedings of the 2014 March Meeting of the American Physical Society. Available on-line at: <http://meetings.aps.org/Meeting/MAR14/Session/F1.3>.

40 **Title of the work:** Study of the Influence of Localized Vibrational Modes in Charge Transport Properties at Nanoscale Systems
Name of the conference: XXXVI ENFMC Brazilian Physical Society Meeting 2013
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
City of event: Águas de Lindóia, Brazil
Date of event: 13/05/2013
End date: 17/05/2013
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo, Brazil
Pedro Brandimarte; Alexandre Reily Rocha; Antônio José Roque da Silva. En: Anais do XXXVI Encontro Nacional de F??sica da Matéria Condensada. Available on-line at: <http://www.sbf1.sbfisica.org.br/eventos/enfmc/xxxvi/sys/resumos/R0970-1.pdf>.

41 **Title of the work:** Study of the role of localized vibrational modes on the charge transport properties at nanoscale systems
Name of the conference: XIII Escola Brasileira de Estrutura Eletrônica
Type of event: Workshop **Geographical area:** National
Type of participation: 'Participatory - poster
City of event: Cuiabá, Brazil
Date of event: 09/07/2012
End date: 13/07/2012
Organising entity: Brazilian Physical Society **Type of entity:** Associations and Groups
City organizing entity: São Paulo,
Pedro Brandimarte; Alexandre Reily Rocha; Antônio José Roque da Silva. En: Anais da XIII Escola Brasileira de Estrutura Eletrônica. Available on-line at: <http://www.fisica.ufmt.br/ebee2012>.

R&D management and participation in scientific committees

Organization of R&D activities

Title of the activity: Towards Reality in Modelling of Molecular Electronics (TRMME)
Type of activity: conference **Geographical area:** Non EU International
City of event: Donostia - San Sebastián, Basque Country, Spain
Convening entity: Donostia International Physics Center **Type of entity:** Research Institute
City convening entity: Donostia - San Sebastián, Basque Country, Spain
Type of participation: Organiser
Start-End date: 13/06/2016 - 17/06/2016 **Duration:** 5 days

Evaluation and revision of R&D projects and articles

1 **Name of the activity:** Reviewer of scientific journal
Performed tasks: Review and evaluation of scientific papers
Entity where activity was carried out: The European Physical Journal
Start date: 17/01/2020

2 **Name of the activity:** Reviewer of scientific journal
Performed tasks: Review and evaluation of scientific papers
Entity where activity was carried out: Journal of Physical Chemistry
Start date: 27/09/2019

3 **Name of the activity:** Reviewer of scientific journal
Performed tasks: Review and evaluation of scientific papers
Entity where activity was carried out: Journal of Physics. Condensed Matter
Start date: 26/01/2017

4 **Name of the activity:** Reviewer of scientific journal
Performed tasks: Review and evaluation of scientific papers
Entity where activity was carried out: ChemistrySelect
Start date: 09/01/2017

5 **Name of the activity:** Reviewer of scientific journal
Performed tasks: Review and evaluation of scientific papers
Entity where activity was carried out: Physica Status Solidi
Start date: 08/12/2016

Other achievements

Obtained grants and scholarships

1 **Name of the grant:** Study of the Influence of Localized Vibrational Modes in Charge Transport Properties at Nanoscale Systems
City awarding entity: São Paulo, Brazil
Aims: Post-doctoral
Awarding entity: National Council of Technological and Scientific Development - CNPq (grant 142792/2010-1)
Type of entity: State agency
Conferral date: 01/10/2010
Duration: 4 years
End date: 01/10/2014
Entity where activity was carried out: São Paulo University
Faculty, institute or centre: Physics Institute

2 **Name of the grant:** ALICE (A Large Ion Collider Experiment) through the HELEN project (High- Energy physics Latin-American European Network)
City awarding entity: Geneva, Switzerland
Aims: Scientific Training
Awarding entity: European Commission, programme América Latina - Formación Académica (ALFA)
Type of entity: Associations and Groups
Conferral date: 01/08/2006
Duration: 6 months
End date: 01/02/2007
Entity where activity was carried out: CERN (Conseil Européen pour la Recherche Nucléaire)

3 **Name of the grant:** Vacuum Quantum Noise Squeezing by Polarization Self-rotation
City awarding entity: São Paulo, Brazil
Aims: Scientific Training
Awarding entity: National Council of Technological and Scientific Development - CNPq (grant 12144/2004-7)
Type of entity: State agency
Conferral date: 01/08/2004
Duration: 1 year
End date: 01/08/2005
Entity where activity was carried out: São Paulo University
Faculty, institute or centre: Physics Institute

Scientific societies and professional associations

1 **Name of the society:** Deutsche Physikalische Gesellschaft
City affiliation entity: Bad Honnef, Köln, Germany
Start date: 2018

2 **Name of the society:** American Physical Society
City affiliation entity: College Park, United States of America
Start date: 2016

3 **Name of the society:** Brazilian Physical Society
City affiliation entity: São Paulo, Brazil
Start date: 2012