CURRÍCULUM VÍTAE NORMALIZADO

José Guilherme Vilhena Albuquerque D'Orey

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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.

To avoid unnecessary repetitions please see the "General quality indicators of scientific research" section for details on number of publications, h index, citations, talks, posters, grants, etc.

My CV demonstrates my capability and a thirst for learning new methods and approaches as needed. I did not keep on publishing on the same research field in which I have started my research career. Instead, I looked for new more challenging problems that fulfilled me as a researcher. I think that the niche of Molecular Dynamics simulations and scanning probe microscopy it is still in its infancy with very little groups in the world working on it. I plan to build my career around this topic, which, as shown by the very productive 2016/2017/2018/2019/2020. Not only there is a high demand from experimental groups for this kind of modeling, but also one is able to publish these results in top journals. This comes driven by the lattest developments in Hardware (GPUs) which nowadays enable us to study a nanoscale systems composed by millions of atoms during microsecond long dynamics. The disadvantage that brought this abrupt change of research field was a very large period of perseverance in the research without any publication. Nevertheless since 2016 this has changed with over 24 publications in only four years and most impressively with a large portion of them in top 10% journals (2Phys.Rev.Lett, 1JACS, 1 ACSNano, 1Nanolett, 1PNAS, 1 Nature Materials, 1 Nat. Comms, 1Nanoscale, 1Carbon). The publication trend clearly shows that it is expectable to keep up the good publication rhythm achieved in 2016, moreover taking into consideration my privileged position as the only modeling researcher in a top experimental research group in nanotribology. As a result of publishing in high impact factor journals my citations are almost doubling each year (2016:22 citations, 2017:51 and 2018:79, 2019:94 see https://scholar.google.com/citations?user=TgoN5scAAAAJ). The change in the research topic, gave me greater maturity and allows me to communicate with many different communities, given the knowledge acquired in ab-initio, Molecular dynamics, biology , friction, surface science and biochemistry communities. In fact, this allowed me to see that the modeling of organic-inorganic friction is still in a very rudimentary level (http://www.pnas.org/content/111/11/3968.abstract), i.e. ball-springs Prandtl-Tomlinson models. The knowledge from biochemistry tools allows me now to simulate bio-molecules with ease. Adding this to my collaborations with the Friction community, in particular with the groups of Ernst Meyer (where I did a stay in Oct/2016), I am now in position to bring a big added value to organic-inorganic friction research field. Furthermore this comes timely with the award of the nobel prize in chemistry of molecular motors, which will certainly ease the publications on this topic. Although risky, and with some personal (as also during these post-doc years I have had 3 sons) and professional cost, this change in the research field provides me a multidisciplinary which I think that is of paramount importance.

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.

OWN FUNDING (Total >370.000€):

> 92.000€ (2019) SNF-SPARK grant where I am the sole PI. This is an excellence grant awarded by the Swiss National Science Foundation to fund the rapid development of new scientific methods, theories, ideas for applications, etc. It is intended for projects that show unconventional thinking and introduce a unique approach. The focus is on promising ideas of high originality.

> 190.000€ (2018) Marie Skłodowska Curie individual fellowship to study molecular friction. My proposal ranked top 2% in the physics evaluation panel.

> 87280€ PhD grant awarded by the "Fundacao para Ciencia e Tecnologia", Portugal. Note that I was the PI of the project/grant, not the PhD supervisor. My research proposal placed second out of 17 grants awarded in the year 2007. The evaluation criteria depend on the student academic grades and proposed research project. This grant gives the flexibility to execute the PhD anywhere in the world.

> Over 2 million CPU hours. I have authored more than 10 computational research projects approved by an international refereeing panel of the "Red Española de Supercomputation-RES" totaling more than 2E6 CPU hours with a total estimated electricity cost >25 000€.

SUPERVISION ACTIVITIES

Co-supervised 2 PhD students (Maria Ortega with Ruben Perez and Alberto Marin Gonzalez with Fernando Moreno and Ruben Perez), two master thesis (Perceval Vellosillo with P. Serena and Maria Ortega Cruz with Ruben Perez) and 1 year secondment (payed for via a National Mexican project written by me and Prof. Serena) of Pamela Rubio Pereda. All students have published at least 1 paper/year in renowned international peer reviewed journals as a result of my close supervision and active participation on the projects.

PUBLICATIONS (source: Scopus)

1) Co-author of 30 peer reviewed research papers:

> 15 as first author or equally contributing with the first;

> 21/30 were published in the last 3 years (including: 2Phys.Rev.Lett, 1Phys.Rev.X, 1JACS,1ACSNano, 1Nanolett, 1PNAS, 1 Nature Materials, 1 Nat. Comms, 1 Nat. Comms.Mat., 2Nanoscale, 1Carbon; 2Nucleic Acids Research);

> in the past 5 years I am publishing >4 articles/year in Q1 peer reviewed journals

> in the past 5 years I am publishing ~3 articles/year in top 10% journals

2) H index of 12, with 345 citations, of which 70% (i.e. 247) were obtained in the past three years. **Please note the trend.**

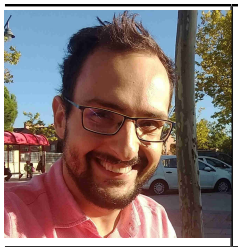
3) Participation in over 40 international conferences via (5 invited talks and over 30 oral contributions). Without counting presentation of my work by others.

4) Publication of 5 press releases as an outreach activity of my research, one of which in "El Mundo".

5) Reviewer in many High Impact journals (SMALL, Nanoscale, ACS Materials, ACS BioMaterials, Carbon,ChemComm, Nanolett ...)

SHORT-TERM RESEARCH STAYS
June/2019 1 week stay in the University of Giessen, Germany. (host: André Schirmeisen)
May/2018&2019 1 month say in the CNR Pisa, Italy. (host: Giacomo Prampolini)
Oct/2016 1 month stay in the University of Basel, Basel, Switzerland. (host: Prof. Ernst Meyer)
Jul/2012 1 month stay in Lawrence Berkeley Laboratory, Berkeley, USA. (host: Prof. M. Salmeron)
Oct/2010 1 week stay in the Aalto University, Helsinki, Finland. (hosts: Prof. R. Nieminen)
Jun/2010 1 week stay in the University of Jyvaskyla, Jyvaskyla, Finland. (host: Prof. Esa Rasanen)

Jun/2009 2 weeks stay in the Univ. Basque Country, San Sebastian, Spain.(host: Prof. Angel Rubio)



José Guilherme Vilhena Albuquerque D'Orey

Surname(s): **Vilhena Albuquerque D'Orey**
Name: **José Guilherme**
ORCID: **0000-0001-8338-9119**
ScopusID: **26023933000**
ResearcherID: **C-6284-2014**
Google Scholar: **https://scholar.google.com/citations?user=TgoN5scAAAAJ&hl=en**

Current professional situation

Employing entity: University of Basel **Type of entity:** University
Department: Nanolino - Meyer group
Professional category: SNF research fellow
Start date: 01/04/2020
Type of contract: Temporary employment contract **Dedication regime:** Full time
Primary (UNESCO code): 120326 - Simulation; 220505 - Friction; 220507 - Measurement of mechanical properties; 230221 - Molecular biology
Secondary (UNESCO code): 221100 - Solid state physics; 221200 - Theoretical physics
Performed tasks: Friction is a phenomenon which is present in our everyday life although we tend to remember it only when it is nearly absent such as when “slipping on a banana peel”. Its presence across disparate length scales (earthquakes, car engines down to molecular machines) reminds us of its ubiquity which endows friction of an utmost practical importance. Therefore, attempts to control it are almost as old as civilization. Interestingly, during the past decades we have witnessed a growing progress in miniaturization of devices down to the nanometer scale. “Special problems occur when things get small [...] and it might turn out to be advantages if we knew how to design for them”, said Feynman when discussing the prospects of building “infinitesimal machinery”. To achieve this goal, and to design efficient molecular nano-engines, it becomes imperative to know how friction at a molecular level can be controlled. I propose to address this challenge by tuning molecular friction and adhesion via atomic/chemical design. Specifically, I study the lifting and sliding of template molecules (porphyrin and terpyridine) over a Gold (111) surface. These molecules contain substituents groups that act as spinning molecular wheels when sliding over a surface. By proper modifications of these groups (wheels) one can tune the grip/drift response and the efficiency of the ball bearing over which the molecular wheel spins. Here I aim to provide an atomic level understanding of these processes by combining state-of-the-art molecular dynamics simulations with high resolution scanning-probe microscopy experiments conducted in ultra-high-vacuum conditions at low temperature. This will constitute a major step forward in our understanding of dissipation processes at the nanoscale and paves the way to tune molecular friction and adhesion by atomic/chemical design.
Identify key words: Peptides and proteins; Nucleotides and nucleosides; Nanostructures; Molecular dynamic; Biophysic chemistry; Stability and folding/ unfolding of proteins

Previous positions and activities

	Employing entity	Professional category	Start date
1	University of Basel	Marie Sklodowska Curie research fellow	01/04/2018

	Employing entity	Professional category	Start date
2	Universidad Autónoma de Madrid	Post-Doc	01/01/2018
3	Centro Nacional de Biotecnología	Post-Doc	01/08/2016
4	Universidad Autónoma de Madrid	Post-Doc	01/08/2015
5	Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)	Post-Doc (Doctor contratado fuera del convenio)	01/03/2013
6	Universidad Autónoma de Madrid	Post-Doc	01/01/2012
7	Laboratoire de Physique de la Matiere Condensee et Nanostructures (LPMCN), Universite Claude Bernard de Lyon 1, Lyon, France	PhD student	01/11/2007

1 **Employing entity:** University of Basel **Type of entity:** University
Department: Nanolino - Meyer group
City employing entity: Basel, Switzerland
Professional category: Marie Sklodowska Curie research fellow
Start-End date: 01/04/2018 - 31/03/2020 **Duration:** 2 years
Type of contract: Temporary employment contract
Dedication regime: Full time
Primary (UNESCO code): 120326 - Simulation; 220505 - Friction; 220507 - Measurement of mechanical properties; 241500 - Molecular biology
Secondary (UNESCO code): 221100 - Solid state physics; 221200 - Theoretical physics
Performed tasks: Friction is a phenomenon which is present in our everyday life although we tend to remember it only when it is nearly absent such as when “slipping on a banana peel”. Its presence across disparate length scales (earthquakes, car engines down to molecular machines) reminds us of its ubiquity which endows friction of an utmost practical importance. Therefore, attempts to control it are almost as old as civilization. Interestingly, during the past decades we have witnessed a growing progress in miniaturization of devices down to the nanometer scale. “Special problems occur when things get small [...] and it might turn out to be advantages if we knew how to design for them”, said Feynman when discussing the prospects of building “infinitesimal machinery”. To achieve this goal, and to design efficient molecular nano-engines, it becomes imperative to know how friction at a molecular level can be controlled. I propose to address this challenge by tuning molecular friction and adhesion via atomic/chemical design. Specifically, I study the lifting and sliding of template molecules (porphyrin and terpyridine) over a Gold (111) surface. These molecules contain substituents groups that act as spinning molecular wheels when sliding over a surface. By proper modifications of these groups (wheels) one can tune the grip/drift response and the efficiency of the ball bearing over which the molecular wheel spins. Here I aim to provide an atomic level understanding of these processes by combining state-of-the-art molecular dynamics simulations with high resolution scanning-probe microscopy experiments conducted in ultra-high-vacuum conditions at low temperature. This will constitute a major step forward in our understanding of dissipation processes at the nanoscale and paves the way to tune molecular friction and adhesion by atomic/chemical design.
Identify key words: Peptides and proteins; Nucleotides and nucleosides; Nanostructures; Molecular dynamic; Biophysic chemistry; Stability and folding/ unfolding of proteins

2 **Employing entity:** Universidad Autónoma de Madrid **Type of entity:** University
Professional category: Post-Doc
Start-End date: 01/01/2018 - 28/02/2018 **Duration:** 2 months
Type of contract: Temporary employment contract

3 **Employing entity:** Centro Nacional de Biotecnología **Type of entity:** State agency
Professional category: Post-Doc

Start-End date: 01/08/2016 - 31/12/2017 **Duration:** 17 months
Type of contract: Temporary employment contract
Dedication regime: Full time
Primary (UNESCO code): 220507 - Measurement of mechanical properties; 241500 - Molecular biology
Secondary (UNESCO code): 221100 - Solid state physics; 221200 - Theoretical physics
Performed tasks: Multiple biological processes involve the stretching of nucleic acids. Stretching forces induce local changes in the molecule structure, inhibiting or promoting the binding of proteins, which ultimately affects their functionality. Understanding how a force induces changes in the structure of nucleic acids at the atomic level is a challenge. In this post-doc I use all atom microsecond-long molecular dynamics to simulate the structure of dsDNA and dsRNA subjected to stretching forces up to 20 pN. Then I was able determine all the elastic constants of dsDNA and dsRNA and provide an explanation for three striking differences in the mechanical response of these two molecules: the three-fold softer stretching constant obtained for dsRNA, the opposite twist-stretch coupling and its non-trivial force dependence. The lower dsRNA stretching resistance is linked with its more open structure, while the opposite twist-stretch coupling of both molecules is traced down to the slide base pair parameter. This parameter affects molecules' radii conferring to dsRNA the unusual property of slightly increasing its radius as it is stretched. This work was published in Proceedings of National Academy of Sciences, one of the top research journals in the field (PNAS 114 (27) 7049-7054). Now I am extending this study to see what is the effect of salt on the mechanical properties of DNA/RNA molecules. Experimentally it has been shown that salt plays an important role leading to a three-fold stiffening of DNA/RNA. Nevertheless there is no explanation, i.e. atomically detailed mechanism, that explains why this happens. I am currently exploring this field. Note that as a consequence of this post-doc I had the opportunity to expand my knowledge into biology. The research group is experimental and has a broad expertise with DNA and DNA interaction with proteins.
Identify key words: Peptides and proteins; Nucleotides and nucleosides; Biophysic chemistry; Stability and folding/ unfolding of proteins

4 **Employing entity:** Universidad Autónoma de Madrid **Type of entity:** University
Department: Department of Theoretical Condensed Matter Physics, Facultad de Ciencias
City employing entity: Madrid, Community of Madrid, Spain
Professional category: Post-Doc **Educational Management (Yes/No):** No
Start-End date: 01/08/2015 - 01/08/2016 **Duration:** 1 year
Type of contract: Temporary employment contract
Dedication regime: Full time
Performed tasks: During this post-doc I was assigned the following tasks: 1) Simulate a friction-force-microscopy measurement in water and in vacuum (ACS nano 10 (4), 4288-4293) ; 2) Co-supervise the Master thesis of Maria Ortega concerning the effect of the inclusion of defects in graphene (Carbon 116, 670 - 677); 3) Simulate friction of a DNA molecule over gold surface (in preparation); 4) Simulate transport through Azurin Cytochrome complex c (under consideration in JACS) ; 5) Measure the mechanical response of antibodies, as measured by AFM (in preparation); 6) Measure and determine the origins for contact frictional ageing (Physical Review Letters 118 (24), 246101 and other work submitted to Nanoletters);
Field of management activity: University
Applicability in teaching and/or research: All these tasks, have one thing in common using classic MD simulations. Each have a given specificity that might be of particular importance. The tasks 1, 3, 4,5 are being done with AMBER software suite. In particular the task 1 and 5 require the use of very complex restrains so to mimic as much as possible an AFM. This restrain control is particularly useful to simulate DNA under given strain. The tasks 3 and 4 required the development of new force-fields parameters (which shall be particularly important if one which to simulate mutations on DNA molecules). The tasks 2, 6 and 7 make use of a different MD engine, i.e. LAMMPS. This not only reflects a high level of maturity in this kind of simulations, but also opens new and interesting avenues. For example, one can easily perform coarse-grained MD simulations with LAMMPS, thus

opening the possibility of simulating much larger molecules (on a similar size as the ones used in the experiments) while retaining a high accuracy and a high level of detailed description of the system. In the task 4, the major goal in a long run is to couple QM simulations with classic MD simulations, thus paving the way to simulate the breaking and repair of chemical bounds.

5 **Employing entity:** Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC) **Type of entity:** Public Research Body

Department: Instituto de Ciencia de Materiales de Madrid

City employing entity: Madrid, Community of Madrid, Spain

Professional category: Post-Doc (Doctor contratado fuera del convenio) **Educational Management (Yes/No):** No

Email: guilhermevilhena@uam.es

Start-End date: 01/03/2013 - 31/07/2015 **Duration:** 2 years - 4 months

Type of contract: Temporary employment contract

Dedication regime: Full time

Primary (UNESCO code): 220600 - Molecular physics; 221032 - Thermodynamics; 230200 - Biochemistry

Performed tasks: This work is performed in the context of Consolider research project Force-For-Future (FFF,CSD2010-00024). [Further details see 1 st post-doc]. During the period in which I was contracted I was assigned the following tasks: 1) Co-supervise the master thesis of Perceval Vellosillo; 2) Co-Supervise the one year stay of the PhD student Pamela Rubio; 3) Perform MD simulations in order to gain a deeper understanding of protein adsorption process to solid surfaces. The first two tasks consisted in training Perceval Vellosillo and Pamela Rubio so to use AMBER software suite to perform MD simulations in a high-performance computing environment. With this knowledge P. Vellosillo was able to contribute to a research article in a prestigious journal (Langmuir 32 - 7, pp. 1742 – 1755 ; 2016) in the field. P. Rubio, already at a more mature stage of her research, was able to actively contribute to two different works (Journal of Chemical Theory and Computation 10 (5), 1837–1842 and Langmuir 32 - 7, pp. 1742 – 1755 ; 2016). All these works, as well as the ones performed only by myself considered the problematic of studying the adsorption of proteins to surfaces under different conditions (ionic strength, presence of step edges, diffusion barriers over step edges; suitability of different solvation models to study protein adsorption and evaluation of free energies of adsorption and diffusion). The complexity of all these works lead to a deeper understanding of all-atom MD methods, in particular free energy methods (Jarzynski and Umbrella sampling) as well as complex solvation methods.

Identify key words: Peptides and proteins; Biophysic chemistry; Stability and folding/ unfolding of proteins

Applicability in teaching and/or research: Here I was able to extend my capabilities on MD simulations as well as to learn how to co-supervise students.

6 **Employing entity:** Universidad Autónoma de Madrid **Type of entity:** University

Department: Departamento de Física Teórica de la Materia Condensada, Facultad de Ciencias

City employing entity: Madrid, Community of Madrid, Spain

Professional category: Post-Doc **Educational Management (Yes/No):** No

Phone: (0034) 914972789 **Fax:** (0034) 914974950 **Email:** guilherme.vilhena@uam.es

Start-End date: 01/01/2012 - 28/02/2013 **Duration:** 1 year - 2 months

Type of contract: Grant-assisted student (pre or post-doctoral, others)

Dedication regime: Full time

Primary (UNESCO code): 220503 - Elasticity; 220505 - Friction; 220507 - Measurement of mechanical properties; 220603 - Macromolecules (physics of); 220609 - Organic molecules; 230221 - Molecular biology; 230223 - Nucleic acids; 230227 - Proteins

Performed tasks: This work took place in the context of a Consolider research project Force-For-Future (FFF,CSD2010-00024). FFF brought together world leading teams on experimental

and theoretical scanning probe microscopy, in order to develop a new generation of scanning probe methods and instruments with applications oriented to nanomechanics and nanomedicine. Therefore, in this context, theory plays a key role in the transition of the newly developed SPM methods to biomedical applications. In particular, given the shear size of the systems (AFM-tip, surface and proteins) the highest level of detail that can be provided though theoretical modeling is though “all-atom” classical force-fields molecular dynamics simulations. Though this contract I was made responsible for performing these simulations. The atomistic information provided by them allow us to convert/understand the experimental data at the nanoscale level into relevant information (mechanical properties, electrical properties, thermal etc). Note that at the time the theoretical modeling of these experiments charted a new, completely unexplored territory: the simulation of high-resolution AFM experiments on biological materials in a liquid environment. In this work, we merge the best knowledge from two, up to now, independent communities. From biophysics, we’ll share the expertise in the atomistic description and full characterization of biological systems. And form the strong theoretical surface science background available at the group of Rubén Peréz we brought the ability to describe and simulate dynamic AFM experiments and extract the relevant sample properties. In the duration of this contract I have performed all-atom MD simulations in order to understand the adsorption process of an antibody to a surface. This work resulted in a publication in a very high impact journal (Nanoscale 8 (27), 13463-13475). Also, during this contract I had the opportunity to co-supervise Maria Ortega's undergrad work, which consisted in applying the same methods I was using to describe the hydration driven mechanical response of single-stranded DNA films (manuscript under preparation). All these research projects were carried out in collaboration with experimental groups (Dr. Ricardo Garcia and Dr. Javier Tamayo respectively) and using well-tested atomistic classical force-fields implemented molecular dynamics codes (AMBER).

Identify key words: Peptides and proteins; Biophysic chemistry; Stability and folding/ unfolding of proteins

Applicability in teaching and/or research: As a consequence of this research contract I had the possibility to extend my knowledge to all-atom classical MD simulations. In particular all the simulations I had performed were done using AMBER software where I learned how to use most of the free energy estimation methods.

7 **Employing entity:** Laboratoire de Physique de la Matiere Condensee et Nanostructures (LPMCN), Universite Claude Bernard de Lyon 1, Lyon, France **Type of entity:** University Research Institute

Department: Laboratoire de Physique de la Matiere Condensee et Nanostructures (LPMCN), Universite Claude Bernard de Lyon 1, Lyon, France, Ecole Doctorale de Physique et d'Astrophysique de Lyon

City employing entity: Lyon, Rhône-Alpes, France

Professional category: PhD student **Educational Management (Yes/No):** No

Phone: (0033) 472448057

Start-End date: 01/11/2007 - 30/11/2011 **Duration:** 4 years

Type of contract: Grant-assisted student (pre or post-doctoral, others)

Dedication regime: Full time

Primary (UNESCO code): 221000 - Physical chemistry; 221100 - Solid state physics

Performed tasks: During the PhD I have worked with a manifold of electronic structure methods. This work followed two main axes: theory/code development and application of these methods to systems of interest. In the first line I have derived the exact conditions obeyed by the exchange and correlation functional for the 2D-electron gas. Using these conditions I have then derived the 2D analogs of the most popular Density-Functional-Theory functionals (PBE, Becke functionals family[B88, B86 and MB86], Colle&Salvetti). Following the theoretical derivation, I also implemented these functionals in a widespread distributed library of exchange and correlation functionals, the LibXC. This enhanced the usage of DFT to describe the 2D-electron gas present in systems such as: modulated semiconductor layers and surfaces, quantum Hall systems, spintronic devices, quantum dots(QDs), quantum rings and artificial graphene. In the second part, devoted to applications, we used a broad spectrum of state-of-the-art ab-initio methods to study the electronic quantum confinement effects (in systems form 1 to 3-dimension: Nanowires, Quantum-Dots and

Transparent-Conducting-Oxides). The methods employed to study these systems were: DFT and GW for the electronic structure; Density Functional Perturbation Theory to access determine phonon dispersions; Random-Phase-Approximation, Time-Dependent-DFT and Bethe-Salpeter equation to determine the optical properties.

Identify key words: Density functional theory; Nanostructures; Nanomaterials

Applicability in teaching and/or research: In the overall, my PhD studies allowed me to get acquainted with state-of-the-art Ab-initio methods, form both developer and an end-user level. I believe that this knowledge is a valuable asset to anyone who wishes to perform theoretical simulations of atomistically detailed processes. The duality of my PhD thesis development/applications allowed me to be aware of the limitations/capabilities of the electronic structure methods thus allowing me to do a better planing, gain a deeper understanding of interactomic interactions and to be able to extend the capabilities of the nowadays very capable commercial/non-comercial simulation suites. Following my PhD, I wished to expand my knowledge beyond electronic structure methods. Although these methods allow us to access a broad range of physical phenomena they are limited not only by the size of the system but also by the time the physical process needs to occur. Electronic structure methods are limited to few thousands of atoms and few hundreds of picoseconds long processes (in the best case scenarios). To overcome this limitation, I have then sought to explore other modeling methods that allowed longer and larger simulations such as all-atom classic Molecular Dynamic simulations. Here I would be able also to profit from the knowledge acquired during the PhD to better understand how these classic inter-atomic potentials are built while being aware of their limitations and scope of validity. This motivated me to expand my knowledge out of my field of comfort thus demonstrating my ability to learn and adapt to new methods as needed.

Education

University education

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

University degree: Higher degree
Name of qualification: Degree in Physics sciences
City degree awarding entity: Coimbra, Centro (P), Portugal
Degree awarding entity: Coimbra University, Portugal **Type of entity:** University
Date of qualification: 20/07/2007

Doctorates

Doctorate programme: First principles study of nano-scale materials: quantum dots and nanowires
Degree awarding entity: Claude Bernard Lyon 1 University, Lyon, France
Date of degree: 19/09/2011

Language skills

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

Teaching experience

General teaching experience

Type of teaching: Official teaching
Name of the course: Laboratory of Physics
Type of programme: Engineering **Type of teaching:** Laboratory work
University degree: Licenciado en Ciencias Químicas Especialidad Ingeniería Química
Start date: 09/2017
Type of hours/ ECTS credits: Credits
Hours/ECTS credits: 24
Entity: Universidad Autónoma de Madrid **Type of entity:** University
Faculty, institute or centre: Chemistry
Department: Chemical engineering
City of entity: Madrid, Spain

Experience supervising doctoral thesis and/or final year projects

1 **Project title:** Combining Molecular Dynamics Simulations and Atomic Force Microscopy Experiments to Rationalize the Mechanical Properties of Double-Stranded DNA and RNA
Type of project: Doctoral thesis
Co-director of thesis: Fernando Moreno Herrero; Ruben Perez Perez; J.G. Vilhena
Entity: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: Alberto Marin Gonzalez
Date of reading: 01/03/2020

2 **Project title:** Tuning dynamical properties of nanoscale systems via atomic-level modifications: insights from all-atom Molecular Dynamics simulations
Type of project: Doctoral thesis
Co-director of thesis: Ruben Perez Perez; J.G. Vilhena
Entity: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Student: Maria Ortega Cruz
Date of reading: 31/01/2020

3 **Project title:** Mentoring the work: Influencia de defectos en la superficie grafítica en el mecanismo de adsorción/difusión de la proteína plasmática más abundante (Albúmina).
Entity: ICMM-CISC [Estancia remunerada durante su doctorado en México (1 year). I have participated as a coauthor and co-supervisor with P. Serena in the research project granted (Clave:393272)]
Student: Yuliana Elizabeth Avila Alvarado
Date of reading: 01/09/2015

4 **Project title:** Mentoring the work: Estudios de la adsorción de la seroalbúmina humana en grafeno: hacia el uso de grafeno en biosensores y bioimplantes
Entity: ICMM-CISC [Estancia remunerada durante su doctorado en México (1 year). I have participated as a coauthor and co-supervisor with P. Serena in the research project granted (Clave: 290749)]
Student: Pamela Rubio
Date of reading: 01/09/2014

5 **Project title:** Mentoring the Master Thesis research project: Hydration properties of single-stranded DNA films: Label-free DNA biosensors, (co-supervised together with Prof. Rubén Pérez)
Entity: Universidad Autónoma de Madrid **Type of entity:** University
Student: María Ortega Cruz
Date of reading: 30/06/2014

6 **Project title:** Mentoring the Master Thesis research project: Atomistic study of adsorption of biomolecules over graphene (P. Vellosillo was hired by Pedro A. Serena for 1 year -2013)
Entity: Universidad Complutense de Madrid **Type of entity:** University
Student: Perceval Vellosillo
Date of reading: 29/01/2014

7 **Project title:** Mentoring the "trabajo de fin de grado": Propiedades de hidratación de una monocapa autoensamblada de hebras de ssDNA mediante dinámica molecular (co-supervised together with Prof. Rubén Pérez)
Entity: Universidad Autónoma de Madrid **Type of entity:** University

Student: María Ortega Cruz
Date of reading: 27/06/2013

Scientific and technological experience

Research and development groups/teams

1 **Name of the group:** Bioelectrochemistry and Nanotechnology Group (FAUSTO SANZ CARRACO research group)
Aims of the group: We are interested in the electronic spectrum of redox capable proteins like Pseudomonas aeruginosa azurin, the electrochemical tunneling spectrum and the energy barrier for single copper protein while their redox state is changed reversibly under potentiostatic control. This work will permit the correlation with reaction rates of specific mutant proteins under different experimental conditions, investigate the mechanism of electron transfer, including long-range electron tunneling and possible gating processes which are not well understood. This method will also be useful to explain the catalytic properties of multi-copper proteins, and will have an impact in the development and optimization of biosensors.
Affiliation entity: Universitat de Barcelona **Type of entity:** University
Start date: 15/12/2016

2 **Name of the group:** Nano Functionality Integration Group (Shigeki Kawai reasearch group)
Aims of the group: Nanomanipulation and Friction at the nanoscale.
Affiliation entity: National Institute for Materials Science **Type of entity:** Public Research Body
Start date: 20/10/2016

3 **Name of the group:** Molecular Biophysics of DNA repair nanomachines (Fernando Moreno-Herrero research group)
Aims of the group: We are interested in studying dsDNA break repair and Chromosome organisation at the single molecule level using Atomic Force Microscopy, Magnetic and Optical Tweezers, and standard biochemical techniques.
Affiliation entity: Centro Nacional de Biotecnologia (CNB-CSIC) **Type of entity:** Public Research Body
Start date: 01/08/2016

4 **Name of the group:** Nanolino Lab (Ernst Meyer research group)
Aims of the group: Our research interest focuses on the structure of insulating surfaces, molecular layers on insulating surfaces, nanotribology, and instrumental development of force microscopy.
Affiliation entity: University of Basel **Type of entity:** University
Start date: 20/01/2016

5 **Name of the group:** Research Group Prof. Dr. André Schirmeisen: Atomic Force Microscopy and Nanotribology
Affiliation entity: Institut fur Angewandte Physik, Justus-Liebig-University Giessen **Type of entity:** University
Start date: 15/10/2015

6 **Name of the group:** Mechanics of functional Materials group (Enrico Gnecco research group)
Aims of the group: The Mechanics of functional Materials group at FSU Jena is investigating several mechanical properties of surfaces at the nanometer scale. Especially interesting for us are friction, wear and adhesion processes on natural and artificial materials. State-of-the art atomic force microscopy is dedicated to this goal.
Affiliation entity: Friedrich-Schiller-University Jena **Type of entity:** University
Start date: 01/01/2015

7 **Name of the group:** Nanoforces group (Julio Gomez-Herrero research group)
Aims of the group: Modelling of different prIn the Nanoforces group we explore the nanoworld using Atomic Force Microscopy as our main tool.oblems in Materials Science and Nanotechnology that involve forces and currents at the atomic scale. In particular, we try to understand and develop new capacities for the basic tools in Nanotechnology, the Scanning Probe Microscopes (SPMs), that enable us to use currents and forces to visualize and manipulate matter at the nanoscale.
Type of collaboration: Co-authorship of publications
Affiliation entity: Universidad Autónoma de Madrid **Type of entity:** University
Start date: 01/01/2014

8 **Name of the group:** FORCETOOL: Advanced Force Microscopy and Nanolithography Lab (Ricardo Garcia research group)
Aims of the group: A combined theoretical and experimental approach to develop multipurpose tools for quantitative analysis and manipulation of molecules, materials and devices in the 1 to 100 nm length scale. A key feature the groups approach is that nanoscale control and device performance should be compatible with operation in technological relevant environments (air or liquids). The group has contributed to the development, understanding and optimization of amplitude modulation AFM (tapping mode). Currently, it participates in the development of bimodal AFM as a unifying scheme for topography and quantitative mapping of material properties with sub-1 nm resolution.
Type of collaboration: Co-authorship of publications
Affiliation entity: Instituto de Ciencia de Materiales de Madrid **Type of entity:** State agency
Start date: 03/06/2013

9 **Name of the group:** Theory and Simulation of Materials
Aims of the group: The goal is to study new properties of modern materials and devices from a theoretical point of view. We aim at understanding experimental data and making experimental predictions, with the major goal of being able to quickly react to new developments and to tackle novel materials and problems in a very agile way.
Type of collaboration: Co-authorship of publications
Affiliation entity: Instituto de Ciencia de Materiales de Madrid **Type of entity:** State agency
Start date: 01/04/2013

10 **Name of the group:** Scanning Probe Microscopy Theory group (Rubén Peréz research group)
Aims of the group: Modelling of different problems in Materials Science and Nanotechnology that involve forces and currents at the atomic scale. In particular, we try to understand and develop new capacities for the basic tools in Nanotechnology, the Scanning Probe Microscopes (SPMs), that enable us to use currents and forces to visualize and manipulate matter at the nanoscale.
Type of collaboration: Co-authorship of publications
Affiliation entity: Universidad Autónoma de Madrid **Type of entity:** University
Start date: 02/01/2012

11 **Name of the group:** Quantum Control and Dynamics (Esa Rasanen research group)
Aims of the group: Our main focus is on quantum phenomena in atoms, molecules, solids, and two-dimensional nanostructures.
Affiliation entity: Tampere University of Technology **Type of entity:** University
Start date: 01/06/2009

12 **Name of the group:** Stefano Pittalis reseach group
Aims of the group: Development and application of computational methods for the simulation of equilibrium and non-equilibrium properties of quantum systems on the nanoscale.
Type of collaboration: Co-authorship of publications

Affiliation entity: Consiglio Nazionale delle Ricerche (CNR-Modena) **Type of entity:** Public Research Body
Start date: 05/01/2009

Scientific or technological activities

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

1 **Name of the project:** Molecular Nanorovers: A roadmap to molecular superlubricity
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Non EU International
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: University of Basel
City of entity: Basel, Switzerland
Name principal investigator (PI, Co-PI....): J.G. Vilhena
Nº of researchers: 1 **Nª people/year:** 1
Name of the programme: SPARK
Start-End date: 01/03/2020 - 28/02/2021 **Duration:** 1 year
Total amount: 92.163 €
Dedication regime: Full time

2 **Name of the project:** Molecular Nano Tribology, Marie Sklodowska Curie individual fellowship project
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** European Union
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: University of Basel **Type of entity:** University
City of entity: Basel, Switzerland
Name principal investigator (PI, Co-PI....): J.G. Vilhena
Nº of researchers: 1
Start-End date: 01/04/2018 - 31/03/2020 **Duration:** 2 years
Total amount: 187.420 €
Dedication regime: Full time

3 **Name of the project:** Hydration Properties of Single-Stranded DNA Films
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Name of the programme: Red Española de supercomputación
Code according to the funding entity: QCM-2016-1-0028
Start-End date: 01/03/2016 - 30/06/2016 **Duration:** 4 months
Total amount: 2.720,34 €
Applicant's contribution: Supervised by Professor Ruben Perez, I have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 238 000 CPU hours and we were granted 180 000 CPU hours due to reduction on all the projects motivated by maintenance of the machine. The RES estimated cost for this project (considering only the electricity cost) is of 2720.34 euros. Aside form actively taking part in the elaboration of the project, I shared this computational resources with the Master student Maria Ortega.

4 **Name of the project:** Atomic-Scale Stick-Slip Friction in a Liquid Environment
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Name of the programme: Red Española de supercomputación
Code according to the funding entity: QCM-2016-1-0032
Start-End date: 01/03/2016 - 30/06/2016 **Duration:** 4 months
Total amount: 4.000,5 €
Relevant results: Ongoing project.
Applicant's contribution: Supervised by Professor Ruben Perez, I have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 350 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. The RES estimated cost for this project (considering only the electricity cost) is of 4000.5 euros. Aside form actively taking part in the elaboration of the project, I shared this computational resources with the Master student Maria Ortega.

5 **Name of the project:** Atomic-Scale Stick-Slip Friction in a Liquid Environment
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Name of the programme: Red Española de supercomputación
Code according to the funding entity: QCM-2015-3-0039
Start-End date: 01/11/2015 - 29/02/2016 **Duration:** 4 months
Total amount: 4.366,26 €
Relevant results: Ongoing project.
Applicant's contribution: Supervised by Professor Ruben Perez, we have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 382 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. The RES estimated cost for this project (considering only the electricity cost) is of 4366.26 euros. Aside form actively taking part in the elaboration of the project, I shared this computational resources with the Master student Maria Ortega.

6 **Name of the project:** Tecnologías de microscopía de fuerza para aplicaciones en nanomecánica y nanomedicina
Type of project: Research and development, including transfer **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Name principal investigator (PI, Co-PI....): Ricardo Garcia; Julio Gomez Herrero; Ruben Perez Perez; Agustina Asenjo Barahona; Álvaro Sao Paulo; Jaime Colchero
Nº of researchers: 7
Funding entity or bodies:
Ministerio de Ciencia e Innovación. Investigación **Type of entity:** Government (Public sector)
City funding entity: Madrid, Community of Madrid, Spain

Type of participation: Others
Name of the programme: Consolider research project Force-For-Future
Code according to the funding entity: CSD2010-00024

Start-End date: 01/01/2011 - 31/12/2015 **Duration:** 5 years
Total amount: 3.000.000 €
Dedication regime: Full time
Applicant's contribution: Theory plays a key role in the transition of the newly developed SPM methods to biomedical applications. The atomistic information provided by my simulations allow us to convert/understand the experimental data at the nanoscale level into relevant information (mechanical properties, electrical properties, etc). The theoretical modeling of these experiments charts a new, completely unexplored territory: the simulation of high-resolution AFM experiments on biological materials in a liquid environment. In this work, we merge the best knowledge from two, up to now, independent communities. From biophysics, we'll share the expertise in the atomistic description and full characterization of biological systems. And form the strong theoretical surface science background available at the group of R.P. we bring the ability to describe and simulate dynamic AFM experiments and extract the relevant sample properties. Here, we applied this knowledge to biological samples with particular focused on: [1]Unraveling the mechanism behind protein adsorption to surfaces with atomistically detailed simulations. Applications: Biocompatibility, biosensors, regenerative medicine, etc. [2] Understand, in order to control the behaviour, of DNA-label free biosensing devices. In particular to have a full description of the intrinsically multiscale process behind the operation of these devices. [3]Measuring elastic properties of biological samples (such as proteins) via AFM experiments; [4]Control/Understand how mutations of a selected group (< 60) of amino acids of a virus capsid change its elastic properties by more than 50%; [5]Measuring friction of graphene surfaces embedded in water, and explain the atomic contrast obtained in these AFM experiments (only obtained previously in ultra-high-vacuum experiments); [6]Measuring the dependence of the elastic properties of graphene with very small concentration of defects (~0.1%), and explain how these defects increase the graphene's Young modulus by more than 60% of its original value. Along all the above mentioned research lines, we use atomistic classic potentials codes such as AMBER, NAMD or LAMMPS, that while describing accurately the physical properties of these systems (hydration and mechanical properties), allow us to study these very large scale systems (100.000 - 1.000.000 atoms). In the whole project, I am the only person performing large-scale simulations (>1000 atoms) required to describe the complex large scale biological samples used in the experiments.

7 **Name of the project:** Mechanical properties of biological systems as measured by atomic force microscopy
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Name of the programme: Red Española de supercomputación
Code according to the funding entity: QCM-2014-2-0041
Start-End date: 01/07/2014 - 31/10/2014 **Duration:** 4 months
Total amount: 2.115 €
Applicant's contribution: Supervised by Professor Ruben Perez, we have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 185 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. In our research project we have asked for 45 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. The RES estimated cost for this project (considering only the electricity cost) is of 2115 euros. Aside form actively taking part in the elaboration of the project, I shared this computational resources with the Master student Maria Ortega and with the PhD student Pamela Rubio.

8 **Name of the project:** Adsorption of proteins on defective surfaces with large-scale molecular dynamics simulations
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain

Name of the programme: Red Española de supercomputación
Code according to the funding entity: QCM-2014-1-0023
Start-End date: 01/03/2014 - 30/06/2014 **Duration:** 4 months
Total amount: 514,35 €
Relevant results: To obtain well-ordered immobilized biomaterial arrays for the integration of bio-sensing units in the semiconductor device technology or to better understand protein adsorption onto implant materials based on carbon substrates, certain properties of the substrate surfaces such as surface topography, play a major role in biomedical engineering and biotechnology applications. One main topographical feature is the presence of surface atomic-level structures that in contact with protein solutions of different concentrations show, in accordance with SPM studies, that protein adsorption occurs preferentially along step edges, where a higher chemical reactivity is expected. To address this problem, we have studied the adsorption of the model globular protein BSA onto a graphene surface with topographic features via molecular-dynamics atomistic simulations. The level of detail in our simulations such as the inclusion of explicit solvent, physiological ion concentrations and long time dynamics, allow us to address with better detail this mechanism. Results show that initial protein diffusion toward substrate occurs much faster with the presence of surface atomic-level structures, followed by an initial biased protein diffusion when adsorbed onto atomic structures with sizes over 10A height due to the lack of van der Waals short range interactions. Moreover the low loss in alpha helical contents of BSA adsorbed supports the capability of biofunctionalization of graphene.
Applicant's contribution: Supervised by Professor Ruben Perez, we have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 45 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. In our research project we have asked for 45 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. The total number of hours used was of 177.800 CPU hours, with an RES estimated cost (considering only the electricity cost) of 2032 euros. Aside form actively taking part in the elaboration of the project, I shared this computational resources with the Master students: Maria Ortega, Perceval Vellosillo and Pamela Rubio.

9 **Name of the project:** Accessing multiscale properties of biological systems (DNA, proteins) via large-scale atomistic molecular dynamics.
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Managing coordinator
Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University
City of entity: Madrid, Community of Madrid, Spain
Name principal investigator (PI, Co-PI....): Jose Guilherme Vilhena; Ruben Perez
Nº of researchers: 2
Name of the programme: Red Española de supercomputación
Code according to the funding entity: QCM-2013-3-0017
Start-End date: 01/11/2013 - 28/02/2014 **Duration:** 4 months
Total amount: 2.630,33 €
Relevant results: We have done a comparative study of different solvation models (explicit and implicit) when studying protein adsorption over surfaces. Against many results published at that time, we have shown that implicit solvation model do not accurately reproduce the protein surface interaction, thus leading to protein denaturalization. Furthermore we have also studied the hydration properties of self-assembled single stranded DNA molecules. We have shown that the differential behavior occurring at different hydration levels, mechanism that is behind the operation mode of label-free DNA biosensors, can be fully explained in terms of the hydration layers forming around each of the ssDNA molecules. An attractive regime between the ssDNA is observed at low hydration levels, due to the sharing of H-bounds, and a repulsive regime is observed at higher hydration levels due to the water affinity of these molecules and the dense packing observed in the channels formed between them.
Applicant's contribution: Supervised by Professor Ruben Perez, we have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 231 000 CPU hours and we were granted all that we have asked for,

with very positive comments of the referees. The total number of hours used was of 284.700 CPU hours, with an RES estimated cost (considering only the electricity cost) of 3255 euros. Aside form actively taking part in the elaboration of the project, I shared this computational resources with the Master students: Maria Ortega and Perceval Vellosillo.

10 **Name of the project:** A theoretical study on the adsorption and mechanical properties of the Immunoglobulin G (IgG) - Part2

Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National

Degree of contribution: Managing coordinator

Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University

City of entity: Madrid, Community of Madrid, Spain

Name principal investigator (PI, Co-PI....): Jose Guilherme Vilhena; Ruben Perez

Nº of researchers: 2

Name of the programme: Red Española de Supercomputacion

Code according to the funding entity: QCM-2013-1-0035

Start-End date: 01/07/2013 - 31/10/2013 **Duration:** 4 months

Total amount: 4.171 €

Relevant results: We have shown that, contrary to what had been observed in other more commonly used surfaces such as mica, in graphene the antibodies adsorbed preferentially on a vertical position. This data, validated experimentally, is of great relevance since the vertical orientations are bioactive, and therefore this kind of setup should decrease the signal to noise ratio in Immunoassay biosensing devices.

Dedication regime: Part time

Applicant's contribution: Supervised by Professor Ruben Perez, we have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 360 000 CPU hours and we were granted all that we have asked for, with very positive comments of the referees. Furthermore, in this call we were the largest user of the Spanish fastest GPU machine, and second fastest supercomputer. The total number of hours used was of 365 000 CPU hours, with an RES estimated cost (considering only the electricity cost) of 4171 euros. Aside form actively taking part in the elaboration of the project, I was the only user of the granted resources.

11 **Name of the project:** A theoretical study on the adsorption and mechanical properties of the Immunoglobulin G (IgG)

Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National

Degree of contribution: Managing coordinator

Entity where project took place: Universidad Autónoma de Madrid **Type of entity:** University

City of entity: Madrid, Community of Madrid, Spain

Name principal investigator (PI, Co-PI....): Jose Guilherme Vilhena; Ruben Perez

Nº of researchers: 2 **Nª people/year:** 2

Type of participation: Others

Name of the programme: Red Española de supercomputación

Code according to the funding entity: QCM-2013-1-0015

Start-End date: 01/03/2013 - 30/06/2013 **Duration:** 4 months

Total amount: 3.646 €

Relevant results: We have shown that Graphene is a biocompatible material with the most abundant blood plasma proteins (antibodies and albumin).

Dedication regime: Part time

Applicant's contribution: Supervised by Professor Ruben Perez, we have written the research project in order to gain access to the supercomputing facilities of RES (Red-Espanola-de-Supercomputacion). In our research project we have asked for 252 000 CPU hours and we were granted all that we have asked for,

with very positive comments of the referees. The total number of hours used was of 319 000 CPU hours, with an RES estimated cost (considering only the electricity cost) of 3643 euros. Aside form actively taking part in the elaboration of the project, I was the only user of the granted resources.

12 **Name of the project:** First principles study of nano-scale materials: quantum dots and nanowires
Entity where project took place: Universite Claude Bernard - Lyon1 **Type of entity:** University
City of entity: Lyon, Rhône-Alpes, France
Name principal investigator (PI, Co-PI....): J.G. Vilhena
Nº of researchers: 2
Funding entity or bodies:
Fundaçao para a ciencia e tecnologia **Type of entity:** State agency
City funding entity: Lisbon, Portugal

Start-End date: 01/12/2007 - 19/09/2011
Total amount: 87.280 €

Scientific and technological activities

Scientific production

H index: 14
Date of application: 05/02/2021
Fuente de Indice H: GOOGLE SCHOLAR

Publications, scientific and technical documents

1 J. G. Vilhena; Maria Ortega; Manuel Uhlig; Ricardo Garcia; Ruben Perez. A Practical Guide to Single Protein AFM Nanomechanical Spectroscopy Mapping: Insights and Pitfalls as Unraveled by All-Atom MD Simulations on Immunoglobulin G. ACS sensors. ACS publications, 2021. Available on-line at: <https://pubs.acs.org/doi/10.1021/acssensors.0c02241>.
Type of production: Scientific paper **Format:** Journal
Position of signature: 1
Total no. authors: 5 **Corresponding author:** Yes
Relevant results: Atomic force microscopy is an invaluable characterization tool in almost every biophysics laboratory. However, obtaining atomic/sub-nanometer resolution on single proteins has thus far remained elusive —a feat long achieved on hard substrates. In this regard, nanomechanical spectroscopy mapping may provide a viable approach to overcome this limitation. By complementing topography with mechanical properties measured locally, one may thus enhance spatial resolution at the single-protein level. In this work, we perform all-atom molecular dynamics simulations of the indentation process on a single immunoglobulin G (IgG) adsorbed on a graphene slab. Our simulations reveal three different stages as a function of strain: a noncontact regime—where the mechanical response is linked to the presence of the water environment— followed by an elastic response and a final plastic deformation regime. In the noncontact regime, we are able to identify hydrophobic/hydrophilic patches over the protein. This regime provides the most local mechanical information that allows one to discern different regions with similar height/topography and leads to the best spatial resolution. In the elastic regime, we conclude that the Young modulus is a well-defined property only within mechanically decoupled domains. This is caused by the fact that the elastic deformation is associated with a global reorganization of the domain. Differences in the mechanical response are large enough to clearly resolve domains within a single protein, such as the three subunits forming the IgG. Two events, unfolding or protein slipping, are observed in the plastic regime. Our simulations allow us to characterize these two processes and to provide a strategy to identify them in the force curves. Finally, we elaborate on possible challenges that could hamper the interpretation of such

experiments/simulations and how to overcome them. All in all, our simulations provide a detailed picture of nanomechanical spectroscopy mapping on single proteins, showing its potential and the challenges that need to be overcome to unlock its full potential.

2 Carlos Romero-Muñiz; María Ortega; J. G. Vilhena; Ismael Díez-Perez; Rubén Pérez; Juan Carlos Cuevas; Linda A. Zotti. Can Electron Transport through a Blue-Copper Azurin Be Coherent? An Ab-Initio Study. The Journal of Physical Chemistry C. 125 - 3, pp. 1693 - 1702. ACS publications, 2021. Available on-line at: <https://pubs.acs.org/doi/10.1021/acs.jpcc.0c09364>.

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

Relevant results: Multiple experiments on the electron transport through solid-state junctions based on different proteins have suggested that the dominant transport mechanism is quantum tunneling (or coherent transport). This is extremely surprising given the length of these molecules (2–7 nm) and their electronic structure (mainly comprising very localized molecular orbitals). Overall, this is probably the single most important puzzle in the field of biomolecular electronics and calls for rigorous calculations of the tunneling probability in protein-based junctions. Motivated by these experiments, we tackle here this problem and report a comprehensive theoretical study of the coherent electron transport in metal–protein–metal junctions based on the blue-copper azurin from Pseudomonas aeruginosa, which is the workhorse in protein electronics. More precisely, we focus on single-molecule junctions realized in STM-based experiments and analyze a wide variety of contact scenarios. Our calculations are based on a combination of molecular dynamics simulations and ab initio transport calculations. Our results unambiguously show that when azurin is not deformed and retains its pristine structure, the end-to-end tunneling probability is exceedingly small and does not give rise to any measurable electrical current. On the other hand, we find that much higher tunneling probabilities are possible when either the STM tip (indented from the top) substantially compresses the protein or the protein is contacted sideways, significantly reducing the effective junction length. We also show that in certain configurations, the presence of surrounding water can also increase the conductance but it cannot explain the high conductance values reported experimentally. In all cases, the current is found to flow through the Cu atom of this metalloprotein, although the role of several other levels close to the Fermi energy cannot be ruled out. We remark that we only evaluate the efficiency of coherent transport and the analysis of the relevance of other potential charge-transport mechanisms is out of the scope of our work.

3 Alberto Marin-Gonzalez; Clara Aicart-Ramos; Mikel Marin-Baquero; Alejandro Martín-González; Maarit Suomalainen; Abhilash Kannan; J G Vilhena; Urs F Greber; Fernando Moreno-Herrero; Rubén Pérez. Double-stranded RNA bending by AU-tract sequences. Nucleic Acids Research. 48 - 22, pp. 12917. 2020. Available on-line at: <https://academic.oup.com/nar/article/48/22/12917/6007656>.

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

Relevant results: Sequence-dependent structural deformations of the DNA double helix (dsDNA) have been extensively studied, where adenine tracts (A-tracts) provide a striking example for global bending in the molecule. However, in contrast to dsDNA, sequence-dependent structural features of dsRNA have received little attention. In this work, we demonstrate that the nucleotide sequence can induce a bend in a canonical Watson-Crick base-paired dsRNA helix. Using all-atom molecular dynamics simulations, we identified a sequence motif consisting of alternating adenines and uracils, or AU-tracts, that strongly bend the RNA double-helix. This finding was experimentally validated using atomic force microscopy imaging of dsRNA molecules designed to display macroscopic curvature via repetitions of phased AU-tract motifs. At the atomic level, this novel phenomenon originates from a localized compression of the dsRNA major groove and a large propeller twist at the position of the AU-tract. Moreover, the magnitude of the bending can be modulated by changing the length of the AU-tract. Altogether, our results demonstrate the possibility of modifying the dsRNA curvature by means of its nucleotide sequence, which may be exploited in the emerging field of RNA nanotechnology and might also constitute a natural mechanism for proteins to achieve recognition of specific dsRNA sequences.

4 Sebastian Scherb; Antoine Hinaut; Rémy Pawlak; J.G. Vilhena; Yi Liu; Sara Freund; Zhao Liu; Xinliang Feng; Klaus Müllen; Thilo Glatzel; Akimitsu Narita; Ernst Meyer. Giant thermal expansion of a two-dimensional supramolecular network triggered by alkyl chain motion. Nature Communications Materials. 1 - 8, 2020. Available on-line at: <https://www.nature.com/articles/s43246-020-0009-2>.

Type of production: Scientific paper

Corresponding author: Yes

Relevant results: Thermal expansion, the response in shape, area or volume of a solid with heat, is usually large in molecular materials compared to their inorganic counterparts. Resulting from the intrinsic molecule flexibility,

conformational changes or variable intermolecular interactions, the exact interplay between these mechanisms is however poorly understood down to the molecular level. Here, we investigate the structural variations of a two-dimensional supramolecular network on Au(111) consisting of shape persistent polyphenylene molecules equipped with peripheral dodecyl chains. By comparing high-resolution scanning probe microscopy and molecular dynamics simulations obtained at 5 and 300 K, we determine the thermal expansion coefficient of the assembly of $980 \pm 110 \times 10^{-6} K^{-1}$, twice larger than other molecular systems hitherto reported in the literature, and two orders of magnitude larger than conventional materials. This giant positive expansion originates from the increased mobility of the dodecyl chains with temperature that determine the intermolecular interactions and the network spacing.

5 Alberto Marin-Gonzalez; Cesar Pastrana; Rebeca Bocanegra; A. Martín-González; J.G. Vilhena; Ruben Perez; Borja Ibarra; Clara Aicart-Ramos; Fernando Moreno-Herrero. Understanding the paradoxical mechanical response of in-phase A-tracts at different force regimes. Nucleic Acids Research. 48 - 9, pp. 5024. 2020. Available on-line at: <https://academic.oup.com/nar/article/48/9/5024/5819597>.

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

Relevant results: A-tracts are A:T rich DNA sequences that exhibit unique structural and mechanical properties associated with several functions in vivo. The crystallographic structure of A-tracts has been well characterized. However, the mechanical properties of these sequences is controversial and their response to force remains unexplored. Here, we rationalize the mechanical properties of in-phase A-tracts present in the Caenorhabditis elegans genome over a wide range of external forces, using single-molecule experiments and theoretical polymer models. Atomic Force Microscopy imaging shows that A-tracts induce long-range (~200 nm) bending, which originates from an intrinsically bent structure rather than from larger bending flexibility. These data are well described with a theoretical model based on the worm-like chain model that includes intrinsic bending. Magnetic tweezers experiments show that the mechanical response of A-tracts and arbitrary DNA sequences have a similar dependence with monovalent salt supporting that the observed A-tract bend is intrinsic to the sequence. Optical tweezers experiments reveal a high stretch modulus of the A-tract sequences in the enthalpic regime. Our work rationalizes the complex multiscale flexibility of A-tracts, providing a physical basis for the versatile character of these sequences inside the cell.

6 Alberto Marin-Gonzalez (equally contributing); J.G. Vilhena (equally contributing); Fernando Moreno-Herrero; Ruben Perez. DNA crookedness regulates DNA mechanical properties at short length scales. Physical Review Letters. 122 - 4, pp. 048102. American Physics Society, 2019. Available on-line at: <https://journals.aps.org/prl/accepted/3407eY5eF9f12268572c65406f0f994c378f8dfce>.

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

Total no. authors: 4

Relevant results: Sequence-dependent DNA conformation and flexibility play a fundamental role in specificity of DNA-protein interactions. Here we quantify the DNA crookedness: a sequence-dependent deformation of DNA that consists on periodic bends of the base pair centers chain. Using extensive 100 ?s-long all-atom molecular dynamics simulations, we found that DNA crookedness and its associated flexibility are bijective: unveiling a one-to-one relation between DNA structure and dynamics. This allowed us to build a predictive model to compute stretch from solely structure. Sequences with very little crookedness show extremely high stretching stiffness and have been previously shown to form unstable nucleosomes and promote gene expression. Interestingly, the crookedness can be tailored by epigenetic modifications, known to affect gene expression. Our results rationalize the idea that the DNA sequence is not only a chemical code, but also a physical one that allows to finely regulate its mechanical properties and, possibly, its 3D arrangement inside the cell.

7 Alberto Marin-Gonzalez; J. G. Vilhena; Fernando Moreno-Herrero; Ruben Perez. Sequence-dependent mechanical properties of double-stranded RNA. Nanoscale. 11, pp. 21471 - 21478. The Royal Society of Chemistry, 2019. Available on-line at: <http://dx.doi.org/10.1039/C9NR07516J>.

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

8 Maria Ortega; J.G. Vilhena; Pamela Rubio-Pereda; P.A. Serena; Ruben Perez. Assessing the accuracy of different solvation models to describe protein adsorption. Journal of Chemical Theory and Computation. 15 - 4, pp. 2548 - 2560. American Chemical Society, 2019.

Format: Journal

Corresponding author: Yes

9 Rémy Pawlak (equally contributing); J. G. Vilhena (equally contributing); Antoine Hinaut; Tobias Meier; Thilo Glatzel; Alexis Baratoff; Enrico Gnecco; Rubén Pérez; Ernst Meyer. Conformations and cryo-force spectroscopy of spray-deposited single-strand DNA on gold. Nature communications. 10 - 1, pp. 685. nature publishing group, 2019.
Format: Journal
Relevant results: Cryo-electron microscopy can determine the structure of biological matter in vitrified liquids. However, structure alone is insufficient to understand the function of native and engineered biomolecules. So far, their mechanical properties have mainly been probed at room temperature using tens of pico-newton forces with a resolution limited by thermal fluctuations. Here we combine force spectroscopy and computer simulations in cryogenic conditions to quantify adhesion and intra-molecular properties of spray-deposited single-strand DNA oligomers on Au(111). Sub-nanometer resolution images reveal folding conformations confirmed by simulations. Lifting shows a decay of the measured stiffness with sharp dips every 0.2–0.3?nm associated with the sequential peeling and detachment of single nucleotides. A stiffness of 30–35?N?m?1 per stretched repeat unit is deduced in the nano-newton range. This combined study suggests how to better control cryo-force spectroscopy of adsorbed heterogeneous (bio)polymer and to potentially enable single-base recognition in DNA strands only few nanometers long.

10 Carlos Romero-Muñiz; María Ortega; J. G. Vilhena; Ismael Diéz-Pérez; Juan Carlos Cuevas; Rubén Pérez; Linda A. Zotti. Mechanical Deformation and Electronic Structure of a Blue Copper Azurin in a Solid-State Junction. Biomolecules. 9 - 9, pp. 506. 2019. Available on-line at: <https://www.mdpi.com/2218-273X/9/9/506>. ISSN 2218-273X
Format: Journal

11 Rémy Pawlak (equally contributing); J. G. Vilhena (equally contributing); Philipp D'Astolfo; Xunshan Liu; Giacomo Prampolini; Tobias Meier; Thilo Glatzel; Justin A. Lemkul; Robert Häner; Silvio Decurtins; Alexis Baratoff; Rubén Pérez; Shi-Xia Liu; Ernst Meyer. Sequential Bending and Twisting around C–C Single Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer. Nano Letters. Just Accepted, pp. https://doi.org/10.1021/acs.nanolett.9b04418. 2019. Available on-line at: <https://doi.org/10.1021/acs.nanolett.9b04418>.
Format: Journal
Corresponding author: Yes

12 Matthias Vorholzer (equally contributing); J. G. Vilhena (equally contributing); Ruben Perez; Enrico Gnecco; Dirk Dietzel; Andr\'e Schirmeisen. Temperature Activates Contact Aging in Silica Nanocontacts. Physical Review X. 9, pp. 041045 - 041045. American Physical Society, 2019. Available on-line at: <https://link.aps.org/doi/10.1103/PhysRevX.9.041045>.
Format: Journal

13 Maria Ortega; J. G. Vilhena; Linda A. Zotti; Ismael Díez-Pérez; Juan Carlos Cuevas; Rubén Pérez. Tuning Structure and Dynamics of Blue Copper Azurin Junctions via Single Amino-Acid Mutations. Biomolecules. 9 - 10, pp. 611. 2019. Available on-line at: <https://www.mdpi.com/2218-273X/9/10/611>. ISSN 2218-273X
Format: Journal
Corresponding author: Yes

14 Romero-Muniz, Carlos; Ortega, Maria; Vilhena, J. G.; Diez-Perez, I.; Carlos Cuevas, Juan; Perez, Ruben; Zotti, Linda A.. Ab initio electronic structure calculations of entire blue copper azurins. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 20, 2018. ISSN 1463-9076
DOI: 10.1039/c8cp06862c
PMID: 30489582

15 Vilhena, J. G.; Perez, Ruben. Slippery in every direction. NATURE MATERIALS. 17, 2018. ISSN 1476-1122
DOI: 10.1038/s41563-018-0172-8
PMID: 30250071

16 Vilhena, J. G.; Gnecco, Enrico; Pawlak, Remy; Moreno-Herrero, Fernando; Meyer, Ernst; Perez, Ruben. Stick-Slip Motion of ssDNA over Graphene. JOURNAL OF PHYSICAL CHEMISTRY B. 122, 2018. ISSN 1520-6106
DOI: 10.1021/acs.jpcb.7b06952
PMID: 28945092

17 Rubio-Pereda(equally contributing), Pamela; Vilhena(equally contributing), J. G.; Takeuchi, Noboru; Serena, Pedro A.; Perez, Ruben. Albumin (BSA) adsorption onto graphite stepped surfaces. JOURNAL OF CHEMICAL PHYSICS. 146, 2017. ISSN 0021-9606
DOI: 10.1063/1.4984037
PMID: 28595417

18 Ruiz, Marta P.; Aragones, Albert C.; Camarero, Nuria; Vilhena, J. G.; Ortega, Maria; Zotti, Linda A.; Perez, Ruben; Carlos Cuevas, Juan; Gorostiza, Pau; Diez-Perez, Ismael. Bioengineering a Single-Protein Junction. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. 139, 2017. ISSN 0002-7863
DOI: 10.1021/jacs.7b06130
PMID: 28981262
Source of citations: WOS **Citations:** 8

19 Lopez-Polin, Guillermo; Ortega, Maria; Vilhena, J. G.; Alda, Irene; Gomez-Herrero, J.; Serena, Pedro A.; Gomez-Navarro, C.; Perez, Ruben. Tailoring the thermal expansion of graphene via controlled defect creation. CARBON. 116, 2017. ISSN 0008-6223
DOI: 10.1016/j.carbon.2017.02.021
Source of citations: WOS **Citations:** 8

20 Mazo, Juan J.; Dietzel, Dirk; Schirmeisen, Andre; Vilhena, J. G.; Gnecco, Enrico. Time Strengthening of Crystal Nanocontacts. PHYSICAL REVIEW LETTERS. 118, 2017. ISSN 0031-9007
DOI: 10.1103/PhysRevLett.118.246101
PMID: 28665657
Source of citations: WOS **Citations:** 6

21 Marin-Gonzalez (equally contributing), Alberto; Vilhena (equally contributing), J. G.; Perez, Ruben; Moreno-Herrero, Fernando. Understanding the mechanical response of double-stranded DNA and RNA under constant stretching forces using all-atom molecular dynamics. PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA. 114, 2017. ISSN 0027-8424
DOI: 10.1073/pnas.1705642114
PMID: 28634300
Source of citations: WOS **Citations:** 7

22 Vilhena, J. G.; Dumitru, A. C.; Herruzo, Elena T.; Mendieta-Moreno, Jesus I.; Garcia, Ricardo; Serena, P. A.; Perez, Ruben. Adsorption orientations and immunological recognition of antibodies on graphene. NANOSCALE. 8, 2016. ISSN 2040-3364
DOI: 10.1039/c5nr07612a
PMID: 27352029
Source of citations: WOS **Citations:** 11

23 Vilhena, J. G.; Rubio-Pereda, Pamela; Vellosillo, Perceval; Serena, P. A.; Perez, Ruben. Albumin (BSA) Adsorption over Graphene in Aqueous Environment: Influence of Orientation, Adsorption Protocol, and Solvent Treatment. LANGMUIR. 32, 2016. ISSN 0743-7463
DOI: 10.1021/acs.langmuir.5b03170
PMID: 26799950

Source of citations: WOS **Citations:** 16

24 Vilhena, J. G.; Pimentel, Carlos; Pedraz, Patricia; Luo, Feng; Serena, Pedro A.; Pina, Carlos M.; Gnecco, Enrico; Perez, Ruben. Atomic-Scale Sliding Friction on Graphene in Water. ACS NANO. 10, 2016. ISSN 1936-0851
DOI: 10.1021/acsnano.5b07825
PMID: 26982997
Source of citations: WOS **Citations:** 24

25 Vilhena, J. G.; Rasanen, E.; Marques, M. A. L.; Pittalis, S.. Construction of the B88 Exchange-Energy Functional in Two Dimensions. JOURNAL OF CHEMICAL THEORY AND COMPUTATION. 10, 2014. ISSN 1549-9618
DOI: 10.1021/ct4010728
PMID: 26580514
Source of citations: WOS **Citations:** 9

26 Putaja, A.; Rasanen, E.; van Leeuwen, R.; Vilhena, J. G.; Marques, M. A. L.. Kirzhnits gradient expansion in two dimensions. PHYSICAL REVIEW B. 85, 2012. ISSN 1098-0121
DOI: 10.1103/PhysRevB.85.165101
Source of citations: WOS **Citations:** 18

27 Vilhena, J. G.; Rasanen, E.; Lehtovaara, L.; Marques, M. A. L.. Violation of a local form of the Lieb-Oxford bound. PHYSICAL REVIEW A. 85, 2012. ISSN 1050-2947
DOI: 10.1103/PhysRevA.85.052514
Source of citations: WOS **Citations:** 9

28 Vilhena, Jose G.; Botti, Silvana; Marques, Miguel A. L.. Excitonic effects in the optical properties of CdSe nanowires. APPLIED PHYSICS LETTERS. 96, 2010. ISSN 0003-6951
DOI: 10.1063/1.3368126
Source of citations: WOS **Citations:** 18

29 Rasanen, E.; Pittalis, S.; Vilhena, J. G.; Marques, M. A. L.. Semi-Local Density Functional for the Exchange-Correlation Energy of Electrons in Two Dimensions. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 110, 2010. ISSN 0020-7608
DOI: 10.1002/qua.22604
Source of citations: WOS **Citations:** 9

30 Pittalis, Stefano; Rasanen, Esa; Vilhena, Jose G.; Marques, Miguel A. L.. Density gradients for the exchange energy of electrons in two dimensions. PHYSICAL REVIEW A. 79, 2009. ISSN 1050-2947
DOI: 10.1103/PhysRevA.79.012503
Source of citations: WOS **Citations:** 23

Works submitted to national or international conferences

1 **Title of the work:** Single molecule nanotribology: understanding friction and adhesion at a single molecule level.
Name of the conference: 13th Users Conference of the Spanish Supercomputing Network (RES)
Type of event: Conference
Type of participation: Participatory - invited/keynote talk
Corresponding author: Yes
City of event: Zaragoza, Aragon, Spain
Date of event: 13/09/2019
Organising entity: Spanish Supercomputing Network (RES)
With external admission assessment committee: Yes

2 **Title of the work:** Conformations and cryo-force spectroscopy of spray-deposited single-strand DNA on gold
Name of the conference: Non Contact AFM (NCAFM2019)
Type of event: Conference
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Regensburg, Germany
Date of event: 29/07/2019
Organising entity: University of Regensburg
With external admission assessment committee: Yes

3 **Title of the work:** Single molecule nanotribology: understanding friction and adhesion at a single molecule level
Name of the conference: Molecules at Surfaces (MOLCH 2019)
Type of event: Conference
Type of participation: Participatory - oral communication
Corresponding author: Yes
City of event: Bern, Switzerland
Date of event: 21/06/2019
Organising entity: University of Bern, Dept. Chemistry and Biochemistry
With external admission assessment committee: Yes

4 **Title of the work:** DNA crookedness regulates DNA mechanical properties at short length scales
Name of the conference: DPG-Frühjahrstagung (2019)
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
Corresponding author: Yes
City of event: Regensburg, Germany
Date of event: 31/03/2019
Organising entity: German Physical Society
With external admission assessment committee: Yes

5 **Title of the work:** Single molecule nanotribology: understanding friction and adhesion at a single molecule level.
Name of the conference: DPG-Frühjahrstagung (2019)
Type of event: Conference **Geographical area:** European Union

Type of participation: Participatory - oral communication
Corresponding author: Yes
City of event: Regensburg, Germany
Date of event: 31/03/2019
Organising entity: German Physical Society
With external admission assessment committee: Yes

6 **Title of the work:** "Snake-Like" motion of a single poly-pyrene chain sliding on gold
Name of the conference: Computing pi-Conjugated Compounds
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
Corresponding author: Yes
City of event: Valencia, Valencian Community, Spain
Date of event: 01/02/2019
Organising entity: Universitat de València **Type of entity:** University
With external admission assessment committee: Yes

7 **Title of the work:** Single molecule nanotribology: understanding friction and adhesion at a single molecule level
Name of the conference: Surface Science and Thin Films (SAOG 2019)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication
Corresponding author: Yes
City of event: Fribourg, Switzerland
Date of event: 31/01/2019
Organising entity: Surface Science and Thin Films Community of Switzerland
With external admission assessment committee: Yes

8 **Title of the work:** Conformations and cryo-force spectroscopy of spray-deposited single-strand DNA on gold.
Name of the conference: Beilstein Nanotechnology Symposium 2018: Molecular Mechanisms in Tribology
Type of event: Conference **Geographical area:** European Union
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Potsdam, Germany
Date of event: 02/10/2018
Organising entity: Beilstein
With external admission assessment committee: Yes

9 **Title of the work:** "Snake-Like" motion of of a single poly-pyrene chain sliding on gold
Name of the conference: NC-AFM 2018 (21st international conference on Non-Contact Atomic Force Microscopy)
Corresponding author: Yes
City of event: Porvoo, Finland
Date of event: 17/09/2018
End date: 21/09/2018
Organising entity: Aalto University
J. G. Vilhena.

10 **Title of the work:** Understanding/Tuning the transport properties of biomolecules atom by atom
Name of the conference: CECAM/Psi-k research conference: BioMolecular Electronics
Corresponding author: Yes
Date of event: 27/08/2018
End date: 31/08/2018
Organising entity: Universidad Autónoma de Madrid **Type of entity:** University
City organizing entity: Madrid, Spain
J.G. Vilhena.

11 **Title of the work:** Temperature Scaling of Contact Ageing
Name of the conference: CECAM Workshop: Emergence of surface and interface structure from friction, fracture and deformation
Type of event: Conference
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Lausanne, Switzerland
Date of event: 24/07/2018
Organising entity: CECAM

12 **Title of the work:** Atomistic understanding of the mechanical properties of bio-molecules
Name of the conference: NanoPortugal 2018
Corresponding author: Yes
City of event: Lisbon, Portugal
Date of event: 07/02/2018
End date: 09/02/2018
Organising entity: Universidade Lusofona

13 **Title of the work:** Measuring mechanical properties in liquids using AFM: an atomistic Molecular Dynamics study
Name of the conference: Conference of the solid state physics division of the Spanish Royal Academy of Sciences
City of event: Valencia, Spain
Date of event: 24/01/2018
Organising entity: Spanish Royal Academy of Sciences

14 **Title of the work:** Nanocontacts: from aging to nanomanipulation
Name of the conference: Trends in Nanotribology 2017
Type of event: Conference **Geographical area:** European Union
Type of participation: 'Participatory - poster
City of event: Trieste, Friuli-Venezia Giulia, Italy
Date of event: 26/06/2017
End date: 30/06/2017
Organising entity: International Center for Theoretical Physics **Type of entity:** Public Research Body
City organizing entity: Trieste, Friuli-Venezia Giulia, Italy
With external admission assessment committee: Yes
J.G. Vilhena; Enrico Gnecco; Rubén Peréz. "Nanocontacts: from aging to nanomanipulation".

15 **Title of the work:** Manipulation of organic molecules (ssDNA and pyrene chains) over a gold surface: insights from atomistic MD simulations.
Name of the conference: 7th European Nanomanipulation Workshop

Type of event: Workshop **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Jena, Thüringen, Germany
Date of event: 20/02/2017
End date: 22/02/2017
Organising entity: Friedrich Schiller University Jena **Type of entity:** University
City organizing entity: Jena, Thüringen, Germany
With external admission assessment committee: Yes
J.G. Vilhena; Remy Pawlak; Philipp Gigler; Antoine Hinaut; T. Meier; Th. Glatzel; A. Baratoff; Ernst Meyer; Enrico Gnecco; Rubén Peréz.

16 **Title of the work:** Measuring mechanical properties in liquids using AFM: an atomistic molecular dynamics study
Name of the conference: Fuerzas y Tunel 2016
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - oral communication **Reasons for participation:** Review before acceptance
City of event: Girona, Catalonia, Spain
Date of event: 07/09/2016
End date: 09/09/2016
Organising entity: Institut Català de Nanociència i Nanotecnologia (ICN2) **Type of entity:** Public Research Body
City organizing entity: Barcelona, Catalonia, Spain
J. Guilherme Vilhena; Pedro A. Serena; Rubén Perez.

17 **Title of the work:** Atomic-Scale Sliding Friction on Graphene in Water
Name of the conference: WE-Heraeus-Seminar: Mechanisms of Tribology
Type of event: Seminar
Type of participation: 'Participatory - poster
City of event: Bad Honnef, Germany
Date of event: 29/03/2016
End date: 01/04/2016
Organising entity: Wilhelm and Else Heraeus Foundation
City organizing entity: Wilhelm and Else Heraeus Foundation,
With external admission assessment committee: Yes
Jose Guilherme Vilhena; Pedro Serena; Ruben Perez. Available on-line at: <http://www.tribomechanisms2016.de/>.

18 **Title of the work:** Strong Anchoring and Vertical Adsorption Orientations of Antibodies on graphene
Name of the conference: Biophysics of Proteins at Surfaces: Assembly, Activation, Signaling
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Madrid, Community of Madrid, Spain
Date of event: 13/10/2015
End date: 15/10/2015
Organising entity: Universidad Complutense de Madrid **Type of entity:** University
City organizing entity: Madrid, Community of Madrid, Spain
With external admission assessment committee: Yes
J.G.; A.C.; Elena; Jesus; Pedro A. Serena; Ricardo; Ruben. Available on-line at: <https://www.biophysics.org/2015spain/Home/tabid/5134/Default.aspx>.

19 **Title of the work:** Adsorption Orientations and Immunological Recognition of Antibodies on Graphene
Name of the conference: CECAM-Workshop: Next generation quantum based molecular dynamics: th th challenges and perspectives
Type of event: Workshop **Geographical area:** European Union
Type of participation: 'Participatory - poster
City of event: Bremen, Germany
Date of event: 13/07/2015
End date: 17/07/2015
Organising entity: Bremen University
City organizing entity: Bremen University, Germany
With external admission assessment committee: Yes
J.G.; A.C.; Elena; Jesus; Pedro A. Serena; Ricardo; Ruben. Available on-line at: <http://www.cecam.org/workshop-1193.html>.

20 **Title of the work:** Atomic-scale sliding friction of graphene in water
Name of the conference: The International Conference on Understanding and Controlling Nano and Mesoscale Friction
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Istanbul, Turkey
Date of event: 22/06/2015
End date: 26/06/2015
Organising entity: Mimar Sinan University
With external admission assessment committee: Yes
Jose Guilherme Vilhena; Pedro Serena; Ruben Perez. Available on-line at: <http://www.costnanotribo.org/2015-istanbul-conference>.

21 **Title of the work:** Mechanical properties of antibodies: an atomistic MD and MF-AFM study.
Name of the conference: Fuerzas y Tunel 2014
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: San Sebastian, Basque Country, Spain
Date of event: 27/08/2014
End date: 29/08/2014
Organising entity: Centro de Física de Materiales (CSIC-UPV/EHU) **Type of entity:** Public Research Body
With external admission assessment committee: Yes
J.G.; Pedro A. Serena; Ruben.

22 **Title of the work:** Surface sample interaction in systems of biological interest: An atomistic MD study
Name of the conference: 5th Multifrequency AFM Conference
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Madrid, Community of Madrid, Spain
Date of event: 16/06/2014
End date: 18/06/2014
Organising entity: CSIC: Instituto de Ciencia de Materiales de Madrid **Type of entity:** Public Research Body
City organizing entity: Madrid, Community of Madrid, Spain
With external admission assessment committee: Yes
J.G.; A.C; Elena; Jesus; Pedro A. Serena; R.; Ruben.

23 **Title of the work:** Friction of graphene immersed in water as measured by AFM: An atomistic theoretical description
Name of the conference: The First European Workshop on Understanding and Controlling Nano and Mesoscale Friction
Type of participation: Participatory - oral communication
City of event: Can Picafort, Mayorca, Spain
Date of event: 26/05/2014
End date: 29/05/2014
Organising entity: FUNDACIÓN IMDEA NANOCIENCIA
With external admission assessment committee: Yes
Jose Guilherme Vilhena; Pedro Serena; Ruben Perez.

24 **Title of the work:** Antibody adsorption over graphene : an atomistic MD and MF-AFM study
Name of the conference: 11th Annual International Workshop on Nanomechanical Sensing (NMC 2014)
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Madrid, Community of Madrid, Spain
Date of event: 30/04/2014
End date: 02/05/2014
Organising entity: Institute of Microelectronics-Madrid (IMM, CSIC) **Type of entity:** Public Research Body
City organizing entity: Madrid, Community of Madrid, Spain
J.G.; A.C.; Elena; Jesus; Pedro A. Serena; Ricardo; Ruben.

25 **Title of the work:** Antibody adsorption over graphene: an atomistic MD and MF-AFM study
Name of the conference: NanoSpain 2014
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Madrid, Community of Madrid, Spain
Date of event: 11/03/2014
End date: 14/03/2014
Organising entity: FUNDACION PHANTOMS
City organizing entity: Madrid, Community of Madrid, Spain
J.G.; A.C.; Elena; Jesus; Pedro A. Serena; Ricardo; Ruben.

26 **Title of the work:** Antibody adsorption over graphene: an atomistic MD and MF-AFM study
Name of the conference: VI International Conference BIFI 2014 "Exploring the role of computation in science: From Physics to Biology"
Type of participation: Participatory - oral communication
City of event: Zaragoza, Spain
Date of event: 22/01/2014
End date: 24/01/2014
Organising entity: Universidad de Zaragoza **Type of entity:** University
City organizing entity: Zaragoza, Spain
Jose Guilherme Vilhena; Andra Dumitru; Elena Tomas Herruzo; Jesus Ignacio Mendieta Moreno; Pedro Serena; Ricardo Garcia; Ruben Perez.

27 **Title of the work:** Molecular dynamics study of the IgG adsorption on a graphene surface
Name of the conference: 15th Linz winterworkshop: Advances in Single-Molecule Research for Biology & Nanoscience

Type of participation: Participatory - oral communication
City of event: Linz, Austria
Date of event: 15/02/2013
End date: 18/02/2013
Organising entity: Johannes Kepler Universitat Linz **Type of entity:** University
City organizing entity: Linz, Austria
Jose Guilherme Vilhena; Elena Tomas Herruzo; Jesus Ignacio Mendieta Moreno; Pablo Pou; Pedro Serena; Ricardo Garcia; Ruben Perez.

28 **Title of the work:** Molecular dynamics study of the IgG adsorption on a graphene surface
Name of the conference: NanoPT2013: Nanoscience and Nanotechnology international conference
Type of participation: Participatory - oral communication
City of event: Oporto, Portugal
Date of event: 13/02/2013
End date: 15/02/2013
Organising entity: FUNDACION PHANTOMS
Jose Guilherme Vilhena; Elena Tomas Herruzo; Jesus Ignacio Mendieta Moreno; Pablo Pou; Pedro Serena; Ricardo Garcia; Ruben Perez.

29 **Title of the work:** Towards a molecular dynamics description of the mechanical properties of antibodies as mesured with atomic force microscopy
Name of the conference: 4th Multifrequeny AFM conference
Type of participation: 'Participatory - poster
City of event: Madrid, Community of Madrid, Spain
Date of event: 15/10/2012
End date: 17/10/2012
Organising entity: Instituto de Microelectrónica de Madrid-CSIC **Type of entity:** Public Research Body
City organizing entity: Spain
Jose Guilherme Vilhena; Pedro Serena; Ricardo Garcia; Ruben Perez.

30 **Title of the work:** Towards a molecular dynamics description of the mechanical properties of antibodies as mesured with atomic force microscopy
Name of the conference: NANOTECHNOLOGY CONFERENCE - FUERZAS Y TUNEL 2012
Type of participation: 'Participatory - poster
City of event: San Lorenzo de El Escorial, Community of Madrid, Spain
Date of event: 12/09/2012
End date: 14/09/2012
Organising entity: Sociedad de microscopia de España
Jose Guilherme Vilhena; Pedro Serena; Ricardo Garcia.

31 **Title of the work:** Ab initio computation of the optical properties of semiconducting nanowires
Name of the conference: Invited Seminar in the Department of Applied Physics, Aalto University School of Science and Technology
Type of participation: Participatory - invited/keynote talk
City of event: Helsinki, Finland
Date of event: 04/10/2010
Organising entity: Department of Applied Physics, Aalto University School of Science and Technology **Type of entity:** University
City organizing entity: Helsinki, Finland
Jose Guilherme Vilhena.

32 **Title of the work:** Excitonic effects in the optical properties of CdSE nanowires
Name of the conference: Nanowires 2010 (NW2010)
Type of participation: Participatory - oral communication
City of event: Heracklion, Creta, Greece
Date of event: 27/09/2010
End date: 01/10/2010
Organising entity: CECAM workshop programme
Jose Guilherme Vilhena; Silvana Botti; Miguel Alexandre Lopes Marques.

33 **Title of the work:** Excitonic effects in the optical properties of CdSE nanowires
Name of the conference: Psi- K 2010
Type of participation: 'Participatory - poster
City of event: Berlin, Germany
Date of event: 12/09/2010
End date: 16/09/2010
Organising entity: Psi-K network
Jose Guilherme Vilhena; Silvana Botti; Miguel Alexandre Lopes Marques.

34 **Title of the work:** Development of exchange and correlation functionals for the 2D electron gas
Name of the conference: Invited seminar Department of Physics, University of Jyvaskyla
Type of participation: Participatory - invited/keynote talk
City of event: Jyvaskyla, Finland
Date of event: 22/06/2010
Organising entity: Nanoscience Center and Department of Physics, University of Jyva?skyla?
City organizing entity: Jyva?skyla?, Finland
Jose Guilherme Vilhena.

35 **Title of the work:** An introduction to Quantum Monte Carlo Methods
Name of the conference: Laboratoire de Physique de la Matiere Condensee et Nanostructures seminars
Type of participation: Participatory - oral communication
City of event: Lyon, France
Date of event: 26/05/2010
Organising entity: Laboratoire de Physique de la Matiere Condensee et Nanostructures, Lyon University
City organizing entity: Lyon, France
Jose Guilherme Vilhena.

36 **Title of the work:** Density Gradients for the exchange energy of electrons in two dimensions
Name of the conference: EFTS 2009: Ab-initio tools for the characterization of nanostructures
Type of participation: 'Participatory - poster
City of event: Evora, Portugal
Date of event: 14/09/2009
End date: 19/09/2009
Organising entity: EFTS
Jose Guilherme Vilhena; Esa Rasanen; Stefano Pittalis; Miguel Alexandre Lopes Marques.

37 **Title of the work:** Density Gradients for the exchange energy of electrons in two dimensions
Name of the conference: Gordon Research conferences: Time-Dependent Density- Functional Theory
Type of participation: 'Participatory - poster
City of event: New London, NH (USA), United States of America
Date of event: 05/07/2009
End date: 10/07/2009

Organising entity: Gordon Research conferences
City organizing entity: New London, NH (USA), United States of America
Jose Guilherme Vilhena; Esa Rasanen; Stefano Pittalis; Miguel Alexandre Lopes Marques.

38 **Title of the work:** First principles studies of optical absorption in nanostructures
Name of the conference: Laboratoire de Physique de la Matiere Condensee et Nanostructures, Lyon University seminars
Type of participation: Participatory - oral communication
City of event: Lyon, France
Date of event: 12/01/2009
Organising entity: Laboratoire de Physique de la Matiere Condensee et Nanostructures, Lyon University
City organizing entity: Lyon, France
Jose Guilherme Vilhena.

39 **Title of the work:** Excitonic effects on CdSe nanowires
Name of the conference: 13th ETSF/Nanoquanta Conference - Theoretical Spectroscopy and Quantum Transport
Type of participation: 'Participatory - poster
City of event: Pugnochiuso, Italy
Date of event: 22/09/2008
End date: 27/09/2008
Organising entity: ETSF
City organizing entity: Pugnochiuso, Italy
Jose Guilherme Vilhena; Silvana Botti; Miguel Alexandre Lopes Marques.

40 **Title of the work:** Excitonic effects on CdSe nanowires
Name of the conference: Time dependent Density- Functional Theory: Prospects and Applications (3rd International Workshop and School)
Type of participation: 'Participatory - poster
City of event: Benasque, Spain
Date of event: 31/08/2008
End date: 15/09/2008
Organising entity: FUNDACION CENTRO DE CIENCIAS DE BENASQUE
City organizing entity: Benasque, Spain
Jose Guilherme Vilhena; Silvana Botti; Miguel Alexandre Lopes Marques.

41 **Title of the work:** Development of two dimensional exchange and correlation functionals
Name of the conference: Journee des doctorants du Laboratoire de Physique de la Matiere Condensee et Nanostructures
Type of participation: Participatory - oral communication
City of event: Lyon, France
Date of event: 17/07/2008
Organising entity: Laboratoire de Physique de la Matiere Condensee et Nanostructures
City organizing entity: Lyon, France
Jose Guilherme Vilhena; Miguel Alexandre Lopes Marques.

Works submitted to national or international seminars, workshops and/or courses

1 **Title of the work:** Single molecule nanotribology: understanding friction and adhesion at a single molecule level.
Type of event: Seminar
Corresponding author: Yes
City of event: Giessen, Germany
Date of event: 25/06/2019
Organising entity: University Justus Liebig Giessen

2 **Title of the work:** Mechanical properties at nanoscale: an atomistic MD description
City of event: Basel, Switzerland
Date of event: 10/2016
Organising entity: Department of Physics, University of Basel

3 **Title of the work:** Mechanical properties of antibodies as measured by AFM: an atomistic Molecular Dynamics study
City of event: Madrid, Spain
Date of event: 10/2015
Organising entity: Fundacion Centro Nacional de Investigaciones Cardiovasculares Carlos III

4 **Title of the work:** Antibody adsorption over graphene: an atomistic MD study
City of event: Berkeley, United States of America
Date of event: 07/2012
Organising entity: Lawrence Berkeley Laboratory

5 **Title of the work:** Excitonic effects in the optical properties of CdSe nanowires
City of event: Helsinki, Finland
Date of event: 10/2010
Organising entity: Aalto University

6 **Title of the work:** Excitonic effects in the optical properties of CdSe nanowires
City of event: San Sebastian,
Date of event: 06/2009
Organising entity: University of the Basque Country

7 **Title of the work:** Construction exchange-correlation functionals for the 2DEG
City of event: Jyvaskyla, Finland
Organising entity: University of Jyvaskyla

Other achievements

Stays in public or private R&D centres

1 **Entity:** University Justus Liebig Giessen **Type of entity:** University
Faculty, institute or centre: Department of Physics
City of entity: Giessen, Germany
Start-End date: 24/06/2019 - 30/06/2019 **Duration:** 7 days
Goals of the stay: Establish novel collaborations with experimental groups
Provable tasks: Understanding friction and contact aging in nanoscale contacts

2 **Entity:** University of Basel **Type of entity:** University
Faculty, institute or centre: Physics Department, Ernst Meyer research group
City of entity: Basel, Switzerland
Start-End date: 01/10/2016 - 01/11/2016 **Duration:** 1 month - 1 day
Funding entity: European Union
Name of programme: COST-MP1303
Goals of the stay: Scientific colaboration
Provable tasks: Lay basis for a solid collaboration with the research group of Professor Ernst Meyer in the topic of molecular Friction.
Acquired skills developed: As a result of this research stay we are actively collaborating on three different works concerning molecular friction, which we expect to have them published during the year of 2017. Furthermore, this laid basis for a longer collaboration in which we shall now write common EU projects.
Relevant results: Stick-Slip firction of DNA over Graphene, sequence dependent response and superlubricity of DNA over graphene. Unraveled the friction mechanisms of pyrene over gold111. This last point revealed that for the first time one is able to extract information about the internal structure of a molecule simply through its friction response. At last we also started a collaboration on high resolution imaging (coupled with our MD simulations) of the canonical protein used in "protein-electronics" so to carachterize for the first time how the contact between the protein and the surface is established.

3 **Entity:** Lawrence Berkeley National Laboratory (invited)
City of entity: Berkeley, United States of America
Start-End date: 28/07/2012 - 28/08/2012 **Duration:** 1 month
Goals of the stay: Scientific collaboration

4 **Entity:** Aalto University (Invited)
City of entity: Aalto, Finland
Start-End date: 04/10/2010 - 08/10/2010 **Duration:** 5 days
Goals of the stay: Scientific Colaboration

5 **Entity:** University of Jyvaskyla (invited)
Faculty, institute or centre: Department of Physics
City of entity: Jyvaskyla, Finland
Start-End date: 21/06/2010 - 25/06/2010 **Duration:** 5 days
Goals of the stay: Scientific Colaboration

6 **Entity:** Nano bio Spectroscopy group, ETSF Scientific Development Center
City of entity: San Sebastian, Spain
Start-End date: 01/06/2009 - 12/06/2009 **Duration:** 12 days

Goals of the stay: Scientific collaboration

7 **Entity:** Consiglio Nazionale delle Ricerche
City of entity: Pisa, Italy
Start date: 11/2019 **Duration:** 7 days
Goals of the stay: secondments of my Marie Sklodowska-Curie Action Individual Fellowships
Provable tasks: Development of reliable classical atomic interaction potentials from first principles calculations

8 **Entity:** Consiglio Nazionale delle Ricerche
City of entity: Pisa, Italy
Start date: 05/2019 **Duration:** 1 month
Goals of the stay: secondments of my Marie Sklodowska-Curie Action Individual Fellowships
Provable tasks: Development of reliable classical atomic interaction potentials from first principles calculations

9 **Entity:** Consiglio Nazionale delle Ricerche
City of entity: Pisa, Italy
Start date: 05/2018 **Duration:** 1 month
Goals of the stay: secondments of my Marie Sklodowska-Curie Action Individual Fellowships
Provable tasks: Development of reliable classical atomic interaction potentials from first principles calculations

Obtained grants and scholarships

1 **Name of the grant:** SNSF-Spark (Rapid funding of unconventional ideas)
City awarding entity: Switzerland
Aims: Post-doctoral
Awarding entity: Swiss National Science Foundation **Type of entity:** State agency
Amount of the grant: 92.163 €
Conferral date: 18/11/2019 **Duration:** 1 year
End date: 28/02/2021

2 **Name of the grant:** [COST] Action MP1303 STSM proposal: NANOTRIBOLOGY OF DNA ON GOLD SURFACES
Aims: Collaboration between EU research groups. Note that this grant was awarded via a competitive call. In total the grant was of 2500€.
Awarding entity: European Union through the COST MP1303 Grant Holder at Institute for Molecules and Materials Radboud University Nijmegen The Netherlands **Type of entity:** Public Research Body
Conferral date: 02/08/2016 **Duration:** 1 month
End date: 01/11/2016
Entity where activity was carried out: University of Basel, Switzerland
Faculty, institute or centre: Department of Physics

3 **Name of the grant:** Fundacao para a ciencia e a tecnologia (Bolsa de doutoramento)
Identify key words: Physics - Quantum physics
Aims: Pre-doctoral
Type of entity: State agency

Awarding entity: Fundacao para a ciencia e a tecnologia, Ministerio da ciencia, tecnologia e ensino superior
Amount of the grant: 87.280 €
Conferral date: 01/10/2007 **Duration:** 4 years
End date: 01/10/2011
Entity where activity was carried out: Universite Claude Bernard Lyon1
Faculty, institute or centre: This is a very prestigious grant in Portugal. When I obtained the grant, the total amount of fellowships given in Portugal to pursue a PhD in exact sciences abroad were less then 20(I was 2nd of list)

4 **Name of the grant:** Marie Sklodowska Curie individual fellowship, with my proposal ranking top 2% in the Physics evaluation panel.
Awarding entity: European commission
Conferral date: 01/04/2018 **Duration:** 2 years
Entity where activity was carried out: University of Basel

Prizes, mentions and distinctions

1 **Description:** Marie Sklodowska Curie individual fellowship (top 2% in the physics pannel)
Awarding entity: European Union - Horizon 2020
Conferral date: 09/02/2018

2 **Description:** Best Physics Student of the Coimbra University 2007 Award (Also best student of my promotion)
Awarding entity: Caixa Geral de Depositos and University of Coimbra **Type of entity:** Associations and Groups
City awarding entity: Coimbra, Centro (P), Portugal
Conferral date: 2007

3 **Description:** Participation grant in the Time dependent Density Functional Theory: Prospects and applications (2nd International Workshop and School), Benasque (Spain), thanks to a grant from the organizing committe.
Awarding entity: organizing committe of the Time dependent Density Functional Theory: Prospects and applications (2nd International Workshop and School)
City awarding entity: Benasque, Spain
Conferral date: 2006

4 **Description:** 4 year PhD fellowship. This is a very prestigious grant in Portugal. When I obtained the grant, the total amount of fellowships given in Portugal to pursue a PhD in exact sciences abroad were less then 20. This grant attributed mainly based on the candidates merit, gave me the opportunity to peruse my PhD in any foreign institution I choose.
Awarding entity: Foundation for science and technology of portugal
City awarding entity: Portugal