



<b>Part A. PERSONAL INFORMATION</b>		<b>CV date</b>	Oct 31 2023
First and Familyname		<b>José Enrique Alvarellos Bermejo</b>	
Researchernumbers		Researcher ID	L-7202-2014
		Orcidcode	0000-0003-2184-2787

**A.1. Current position**

Name of University/Institution	Universidad Nacional de Educación a Distancia (UNED)		
Department	Departamento de Física Fundamental. Facultad de Ciencias.		
Current position	Catedrático de Universidad	From	12/01/2010

**A.2. Education**

PhD	University	Year
Ph. D. in Physics	Autonomous University of Madrid	1984

**A.3. JCR articles, h Index, thesis supervised...**

My research activity is reflected in the publication of 46 research articles in relevant international journals, which have received a total of 874 citations (WoS), from 540 articles, with a h index h=16.

The average number of citations per year was about 30 in the last five years.

In addition, I have published a book chapter with research results.

I have been positively evaluated in six research periods, each of six years (sexenios), by the Spanish National Commission of the Research Activity. Last period evaluated: up to 2017.

I have supervised three doctoral theses.

**Part B. CV SUMMARY**

My professional career began in 1977, hired as Teaching Assistant in the Department of Physics of the Autonomous University of Madrid.

In 1980 I was hired by the University of Santiago de Compostela, as Course Professor, for the start-up of the degree in Physical Sciences at that university.

I have been Associate Professor at the Faculty of Physics of the University of Santiago de Compostela (1987-1989) and at the Faculty of Sciences of the National University of Distance Education (UNED, 1989-2010).

I am currently Full Professor in the area of Condensed Matter Physics in the Faculty of Sciences of the UNED (since 2010).

**Research activity.**

My research activity has been reflected in the publication of 46 articles in relevant international journals in the corresponding research fields, which have received a total of 874 citations (WoS) from 540 articles, with the result of an index h equal to 16. I have got the positive evaluation of six research periods, each of six years (sexenios), by the National Commission of the Research Activity. Last period evaluated: up to 2017.

In addition, I have published a book chapter with research results with David García-Aldea.

I have participated as a member of the team of research projects in a number of national and international calls.



I have been a researcher (supported by a one-year NATO fellowship; hired afterwards) at the University of California, Santa Barbara, for 15 months in 1986 and 1987.

I have worked at the Max-Plank-Institut für Festkörperforschung (Stuttgart, RFA) for two months in 1985 and in the Theoretical Chemistry Group of the Faculty of Sciences of the Universidad de los Andes (Mérida, Venezuela) (one month in 1997 and six weeks in 1998, as well as short visits since then).

## Part C. RELEVANT MERITS

### C.1. Publications (including books)

Some of the research works I have published:

Begoña Mula, Eva M. Fernández, **José E. Alvarellos**, Julio J. Fernández, David García-Aldea, Silvia N. Santalla, and Javier Rodríguez-Laguna: Ergotropy and entanglement in critical spin chains, Phys. Rev. B 107, 075116 (2023) [8 pages], DOI: 10.1103/PhysRevB.107.075116

Óscar Toledano, M. Pancorbo, **J. E. Alvarellos** and Óscar Gálvez; Melting in two-dimensional systems: Characterizing continuous and first-order transitions, Phys. Rev. B 103, 094107 (2021) [14 pages], DOI: 10.1103/PhysRevB.103.094107

Eva M. Fernández, Silvia Santalla, **José E. Alvarellos**, Javier Rodríguez-Laguna: Nanowire reconstruction under external magnetic fields, The Journal of Chemical Physics, 153, 244106 (2020) [10 pages], DOI: <https://doi.org/10.1063/5.0031842>

Hernán Santos, **José E. Alvarellos** and Javier Rodríguez-Laguna: Engineering large end-to-end correlations in finite fermionic chains, Phys. Rev. B 98, 245121, DOI: 10.1103/PhysRevB.98.245121

Santos H, Latge A, **Alvarellos JE**, Chico L: All-electrical production of spin-polarized currents in carbon nanotubes: Rashba spin-orbit interaction. Physical Review B **93**, 165424 (2016). DOI: 10.1103 / PhysRevB.93.165424.

Rincon L, **Alvarellos JE**, Almeida R: An analysis of two local measures of the electronic localization: a comparison with the ELF and the exchange-correlation density results. Phys. Chem. Chem. Phys., 2011,13, 9498-9506. DOI: 10.1039/C0CP02711A.

Rincon, Luis; Almeida, Rafael; **Alvarellos, JE**; et al.: The sigma delocalization in planar boron clusters. Dalton Transactions **2009** Issue: 17, 3328-3333 (2009). DOI: 10.1039/b818068g.

García-Aldea D, **Alvarellos JE**: Approach to kinetic energy density functionals: Nonlocal terms with the structure of the von Weizsäcker functional. Phys. Rev. A **77** 022502 (2008).

García-Aldea D, **Alvarellos JE**: Fully nonlocal kinetic energy density functionals: A proposal and a general assessment for atomic systems. J. Chem Phys, **129**, 074103 (2008).

García-Aldea D, **Alvarellos JE**: Kinetic Energy Density Study of Some Representative Semilocal Kinetic Energy Functionals. J. Chem Phys **127**, 144109 (2007).



Jung J; **Alvarellos JE**: Two interacting electrons confined within a sphere: An accurate solution. *Journal of Chemical Physics* **118**, 10825-10834 (2003). DOI: 10.1063/1.1574786.

Garcia-Gonzalez P; **Alvarellos JE** and Chacon E: Nonlocal symmetrized kinetic-energy density functional: Application to simple surfaces. *Physical Review B* **57** (8) , 4857-4862 (1998).

García-Gonzalez P; **Alvarellos JE** and Chacon E: Nonlocal kinetic-energy-density functionals. *Physical Review B* **53**, 9509-9512 (1996).

García-Gonzalez P; **Alvarellos JE** and Chacon E: Kinetic-energy density functional: Atoms and shell structure. *Physical Review A* **54**, 1897-1905 (1996).

Garcia-Aldea D and **Alvarellos JE**: Kinetic energy density study of some representative semilocal kinetic energy functionals. *Journal of Chemical Physics* **127**, 144109 (2007).

**Alvarellos, J**; Metiu, H. The Evolution Of The Wave-Function In A Curve Crossing Problem Computed By A Fast Fourier-Transform Method. *Journal of Chemical Physics*, **88**, 4957-4966 (1988).

Chacon E; **Alvarellos JE** and Tarazona P: Nonlocal Kinetic-Energy Functional For Nonhomogeneous Electron-Systems. *Physical Review B* **32** (12) , pp.7868-7877 (1985).

García-Aldea D, **Alvarellos JE**: "*The construction of kinetic energy functions and the linear response function*", (pp. 290-316, in *Theoretical and Computational Developments in Modern Density Functional Theory*. Editor: Amlan K. Roy. Nova Science Publishers, Inc., NY, USA. (2012). ISBN-13: 978-1619427792. (Book chapter).

## C.2. Research projects and grants

Some of the projects in which I have participated:

1.- Quantum complex systems: fundamentals and applications

Sources of Financing: AEI, reference PID2019-105182GB-I00

Duration: 2020-2023

Principal investigators: Eva M. Fernández Sánchez and J. Rodríguez Laguna (UNED).

1.- Study of the dynamics of complex quantum systems: from fundamental theoretical developments to energy applications (capture, storage, transmission), DYNAPLEX.

Sources of Financing: DGI, reference FIS2010-21282-C02-02.

Duration: 2011-2013. Coordinated with a project of the University of the Basque Country.

Principal investigator: P. García González (UNED).

2.- Applications at the frontier of theoretical spectroscopy: nanostructures and complex systems.

Sources of Financing: DGI, reference FIS2007-65702-C02-02

Duration: 2008-2010

Project coordinated with another from the University of the Basque Country.

Principal investigator: P. García González (UNED).



## C.5. Supervised doctoral theses.

1.- GARCÍA GONZALEZ, Pablo.

Density functional formalism: development of functionals for the kinetic energy of an electron system. June 1997. Extraordinary Doctorate Award (1998).

2.- JUNG WOO, Jeil.

Study of the electronic correlation in simple inhomogeneous systems. May 2005.

European mention. Extraordinary Doctorate Award (2006).

3.- GARCÍA ALDEA, David.

Development and study of kinetic functionals of the electronic density. June 2006.

## C.6. Other activities

### Teaching activity.

I have taught in the first and second cycle of the Physics *licenciatura* (a five-years degree) and in the first cycle of the Chemistry one. I have also taught in the degrees in Physics, in Environmental Sciences, and in Chemistry (all of them Bolonia's four-years degrees). Moreover, in the Master of Physics of Complex Systems, as well as in the third cycle and in the Ph.D. studies in Physics.

I am co-author of five books of teaching character.

I have supervised three doctoral theses, two of them with Extraordinary Prize.

I have been positively evaluated in eight periods of teaching activity (each period, five-years).

### Teaching publications

**J. E. Alvarellos** y J.A.Garzón. *Introducción a la Informática para Científicos*, eds. J.Mira y J.A.Garzón. Editorial: Universidad de Santiago de Compostela (1983), ISBN: 84-300-9493-6. Pages 244-333.

I. Zúñiga, **J. E. Alvarellos** y J. de la Rubia. *Mecánica* (CC. Químicas). Editorial: UNED, Colección Guías Didácticas, 141 pages (1999), ISBN: 84-362-4011-1.

I. Zúñiga, **J. E. Alvarellos** y J. de la Rubia. *Mecánica y Ondas* (CC. Físicas), Editorial: UNED, Colección Guías Didácticas, 152 pages. (1999), ISBN: 84-362-4010-3.

P. García González, **J. E. Alvarellos**, J. J. García Sanz. *Introducción al formalismo de la Mecánica Cuántica*. Editorial: UNED, Colección Cuadernos de la UNED, 262 pages. (1a edición: 2000, 1a edición revisada: 2001), ISBN: 84-362-4137-1.

P. García González, **J. E. Alvarellos**, J. J. García Sanz. *Introducción al formalismo de la Mecánica Cuántica*. (2 edición, 2007). Editorial: UNED, Colección Cuadernos de la UNED, 344 pages, ISBN: 978-84-362-5456-3.

P. García González, **J. E. Alvarellos**, J. J. García Sanz. *Física Cuántica I*. Editorial: UNED, Colección Grado, 447 págs. (2012; séptima reimpresión 2022), ISBN: 978-84-362-6566-8.

### Management and administration

- Vice-Rector of Planning and Infrastructures (UNED) for 3 years (2003-2005)

- Deputy Vice-Chancellor of Infrastructures (UNED), from January 2006 to 2010.

- Chair of the Department of Fundamental Physics of the UNED for 3 years.

- Principal Investigator of MEC research projects for 3 years.



**CURRICULUM VITAE ABREVIADO (CVA)**

**IMPORTANT** – *The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.*

**Part A. PERSONAL INFORMATION**

First name	Eva María		
Family name	Fernández Sánchez	Date:	26/10/2023
ID number			
Open Researcher and Contributor ID (ORCID) (*)		0000-0003-2085-0478	

(\*) Mandatory

**A.1. Current position**

Position	Associate Professor (Titular de Universidad)	
Initial date	30/09/2020	
Institution	Universidad Nacional de Educación a Distancia (UNED)	
Department/Center	Departamento de Física Fundamental	Facultad de Ciencias

**A.2. Previous positions (research activity interruptions, indicate total months)**

Period	Position/Institution/Country/Interruption cause
05/03/2020/29/09/2020	Tenured Professor / UNED / Spain
01/11/2015-04/03/2020	Ramón y Cajal contract / UNED / Spain
01/11/2012-31/10/2015	Postdoc / UNED / Spain
16/03/2008-31/10/2012	Postdoc / Instituto de Ciencia de Materiales de Madrid (ICMM) / Consejo Superior de Investigaciones Científicas (CSIC) / Spain
01/03/2006-29/02/2008	Postdoc / Technical University of Denmark / Denmark
01/01/2002-31/12/2005	Predoc FPU (beca de formación de personal universitario) / Universidad de Valladolid / Spain

**A.3. Education**

PhD, Licensed, Graduate	University/Country	Year
Physics degree	Universidad de Valladolid	2001
Physics PhD	Universidad de Valladolid	2005

(Include all the necessary rows)

**Part B. CV SUMMARY (max. 5000 characters, including spaces)**

- 44 JCR articles (most in Q1). Citations: 2158. H-index: 18
- 5 articles with more than 100 citations.
- PI of a current national project (along with Javier Rodríguez Laguna).
- PI of a research group at UNED.

**Trajectory.** I graduated in Physics at Universidad de Valladolid in 2001. Then I started my research career with a FPU grant from the Spanish Ministry of Science to work on the PhD at the department of “Física Teórica, Atómica y Óptica” at Universidad de Valladolid supervised by Prof. Luis C. Balbás. In December 2005 I obtained the PhD degree with the highest marks. My PhD was awarded Special Doctorate Award by Universidad de Valladolid in 2007. From March 2006 to March 2008 I joined as postdoc at the Technical University of Denmark for two years. From March 2008 to October 2018 I worked as a researcher at Instituto de Ciencia de Materiales de Madrid (ICMM) which is part of the Consejo Superior de Investigaciones Científicas (CSIC), firstly with a JaeDoc Postdoctoral contract and then with a Comunidad de Madrid postdoctoral contract associated to project. Since November 2012 I develop my research work at the department of Física Fundamental of Universidad Nacional de Educación a Distancia, initially with a competitive postdoctoral contract of UNED and since November

2015 with a Ramón y Cajal contract. Finally, I obtained a permanent position in the same department in March 2020.

**Scientific publications.** I have published 44 papers in JCR journals (one Angew. Chem. Int., one Physical Review Letters and seven Physical Review B), which have received more than 1600 citations altogether. Fifteen of my papers have received more than 25 citations (one of them has received more than 490 citations) and my Hirsch index is h=18.

**Funding.** I have participated in 12 research projects, one international project funded by the Danish Research Agency and 6 national projects (one of them in collaboration with Osnabrück University, Germany). At this moment I am PI of a national project (Ref. PID2019-105182GB-I00). In 2017 and in 2019 I was assigned a 1 year undergraduate contract under the competitive Programa de garantía juvenil de la Comunidad de Madrid.

Since 2022 I am evaluator of national project for the Agencia Estatal de Investigación.

**Awards.** I was awarded the L’Oreal-UNESCO prize for Women in Science in Spain 2017, and the Prize of the Real Sociedad Española de Física – Fundación BBA for Young Researchers in theoretical physics in its 21<sup>th</sup> edition (year 2007) in 2008.

**Other contributions.** I am PI of the research group of the Statistical Mechanics of Complex Systems group at UNED.

I have supervised four master thesis and four bachelor thesis.

From 2018 I am an editorial board member for “Revista Española de Física”.

Recently, I have carried out scientific outreach such as giving a conference at the academic act of San Alberto Magno for the Faculty of Science of UNED 2018, giving a Masterclass within the “Stem Talent Girl Proyecto de innovación educativa” program in Valladolid (February 2019) and publishing an article at “Revista Española de Física”.

### **Research lines.**

My research is focused on the analysis of the structural, electronic and thermodynamic properties, by means of first-principles simulation methods, of new tentative materials for applications in catalysis.

I work on two research lines:

#### 1. Nanometric cluster

Improvement and proposal of catalysts for the adsorption of H<sub>2</sub>, O<sub>2</sub>, CO, NO on doped clusters. The main interest is the search for new catalysts more active that reduce air pollutant emissions into the atmosphere and more efficient materials for hydrogen storage. The analysis of the role played by the dopant atom in the reactivity of these aggregates according to their size and composition allows to improve or design new more efficient catalysts for the oxidation of CO and NO *decomposition* (avoiding or reducing their emission to the atmosphere) or for H storage (the main difficulty for the use of hydrogen as an energy source is its storage in a safe, reliable and compact way).

#### 2. Analysis of the liquid-solid interface: the wetting problem in smooth and rough surfaces.

This problem presents a great technological interest as the partial or complete wetting of the surface by the fluid is one of the main influences on a catalyst efficiency. A partial wetting situation, where the fluid only wet a part of the catalyst, implies a low use of the catalyst, as well as the formation of hot spots and, in addition, affects its selectivity.

### **Part C. RELEVANT MERITS (sorted by typology)**

#### **C.1. Publications**

1. E. M. Fernández and L. C. Balbás. *Adsorption of multiple NO molecules on Au<sub>10</sub><sup>-</sup> and Au<sub>9</sub>Zn<sup>-</sup> planar clusters. A comparative DFT study.* Phys. Chem. Chem. Phys. 25, 17176 (2023).

**2.** E. M. Fernández and L. C. Balbás. *Interactions of nitric oxide molecules with pure and oxidized silver clusters  $\text{Ag}_n^{\pm}/\text{Ag}_n\text{O}^{\pm}$  ( $n=11-13$ ): A computational study.* J. of Chem. Phys. 157, 074310 (2022).

In this paper we show that species  $\text{Ag}_n^{\pm}$  and  $\text{Ag}_n\text{O}^{\pm}$  with odd number of electrons are more reactive toward the adsorptions of one and two NO molecules than their neighbors.

**3.** E. M. Fernández, S. N. Santalla, J. E. Alvarellos, J. Rodríguez-Laguna. *Nanowire reconstruction under external magnetic fields.* J. of Chem. Phys. 153, 244106 (2020).

Can nanowires reconstruct differently in the presence of external magnetic (or electric) fields? After our calculations, we can conjecture that this can indeed be the case.

**4.** E. M. Fernández and L. C. Balbás. *Multiple adsorption of molecular oxygen on small Au/Pd cationic clusters at finite temperature. A van der Waals density functional study.* J. of Chem. Phys. 114, 224308 (2016). Citations: 3

The reactivity of  $\text{Au}_n^+$  cluster toward  $\text{O}_2$  is strongly enhanced when Au atoms are changed by Pd ones for all cluster sizes.

**5.** E. Chacón, E. M. Fernández and P. Tarazona. *Effect of dispersion forces on the capillary-wave fluctuations of liquid surfaces.* Phys. Rev. E (89), 042406 (2014) Citations: 12.

Shows molecular dynamics evidence for the nonanalytic effects of the long-range dispersion forces on the capillary waves fluctuations of a Lennard-Jones liquid surface.

**6.** E. M. Fernández, E. Chacón, P. Tarazona, A. O. Parry and C. Rascón. *Intrinsic Fluid Interfaces and Nonlocality.* Phys. Rev. Lett. 111, 096104 (2013) Citations: 21.

Explores the local or nonlocal nature of the interfacial Hamiltonians that are used to analyze the structure and fluctuations of a liquid-gas interface.

**7.** E. M. Fernández, A. Vega and L. C. Balbás. *Theoretical study of  $\text{Al}_n\text{V}^+$  clusters and their interaction with Ar.* J. Chem. Phys. 139, 214305 (2013) Citations: 6.

DFT calculations confirms that the V atoms on  $\text{Al}_n\text{V}^+$  clusters becomes encapsulated at the critical size of 17 atoms as suggested photofragmentation mass experiments.

**8.** E. M. Fernández et. al. (1/11) *Scaling relationships for adsorption energies on transition metal oxide, sulfide, and nitride surfaces.* Ang. Chem. Int. ed. 107, 4683 (2008). Citations: 243. We propose a method that may facilitate the description of the bonding of gas molecules to transition metal oxides, sulfides, and nitrides by density functional theory calculations.

**9.** E. M. Fernández, J. M. Soler and L. C. Balbás. *Planar and cage-like structure of gold clusters: Density-functional pseudopotential calculations.* Phys. Rev. B 73, 235438 (2006). Citations: 107. In this paper we analyze the influence of the exchange-correlation functional (LDA and GGA) in the structure of formation of planar and pure surface (cage-like) clusters.

**10.** E. M. Fernández, J. M. Soler, I. L. Garzón and L. C. Balbás. *Trends in the structure and bonding of noble metal clusters.* Phys. Rev. B 70, 165303-14 (2004). Citations: 492.

Analysis of the differences and similarities between small clusters of noble metals (gold, silver and copper; both neutral and charged).

**C.2. Congress**, indicating the modality of their participation (invited conference, oral presentation, poster)

**1** *Adsorption of multiple NO molecules on  $\text{Au}_{10}^-$  and  $\text{Au}_9\text{Zn}^-$  planar clusters. A comparative DFT study.* ISSPIC XXIII, Berlin, Germany (2023). Poster presentation.

**2.**  *$\text{H}_2$  adsorption on  $\text{Al}_n\text{Co}^+$  clusters.* Gordon Research Conference on Clusters and Nanostructures. Les Diablerets, Switzerland (2019). Poster presentation.

**3.** *Multiple adsorption of molecular oxygen on small Au/Pd cationic clusters at finite temperature. A van der Waals density functional study.* ISSPIC XVIII, Jyvaskyla, Finland (2016). Poster presentation.

4. *Static polarizability of Ar-AuX complexes ( $X = F, Hg$ ) and  $Au_n$  clusters. DFT calculations with a non local correlation van der Waals functional compared to GGA results.* ISSPIC XV, Oaxaca, Mexico (2010). Oral presentation.
5. *Aplicación del ISM al estudio de la transición de mojado.* FISES09, Huelva, Spain (2009). Oral presentation.
6.  *$O_2$  adsorption on cationic gold clusters pure and doped whit a 3d transition metal.* XXX Reunión bienal de la RSEF, Ourense, Spain (2005). Oral presentation.
7. *Theoretical study of  $O_2$  and CO adsorption on gold clusters in gas phase and supported on alumina nano-particles and surfaces.* XXX Reunión bienal de la RSEF, Ourense, Spain (2005). Oral presentation.
8. *Trends in the structure and bonding of pure and doped noble metal clusters. Application to  $O_2$  and CO adsorption.* Quantum system in chemistry & physics, Les Houches, France (2004). invited conference.
9. *Trends in the structure and bonding of neutral and charged noble metal clusters.* Siesta-Meeting, Madrid, Spain (2004). Oral presentation.
10. *Tendencias en la estructura atómica y enlace químico de agregados neutros y cargados de metales nobles.* Segunda reunión mexicana de físico-química teórica, Guanajuato, Mexico (2003). Oral presentation.

**C.3. Research projects**, indicating your personal contribution. In the case of young researchers, indicate lines of research for which they have been responsible.

1. *Quantum Complex Systems: Fundamentals and Applications.* Ministerio de Ciencia, Innovación e Universidades. 06/2019-05/2022 PI: Eva María Fernández (UNED) and Javier Rodríguez-Laguna (UNED) Role: IP1.
2. *Structure and dynamics of complex fluids and their interfaces.* Ministerio de Ciencia e Innovación. 2011-2013; Enrique Chacón Fuertes (CSIC). Researcher.
3. *Structure, dynamics and electronic properties of atomic clusters, nanoalloys, interfaces and metallic liquids of technological interest in spintronics, catalysis and nuclear reactors.* Junta de Castilla y León. 2011-2013. Andrés Aguado Rodríguez (UVa). Researcher.
4. *Modeling and simulation of complex systems.* Comunidad de Madrid. 2010-2013. Enrique Lomba García (CSIC). Researcher.
5. *Electronic and morphological properties of nanostructures materials of interest in spintronics, catalysis and new nanoalloys.* Ministerio de Ciencia e Innovación. 2009-2011. Andrés Vega (UVa). Researcher.
6. *New electrode materials for hydrogen evolution.* Danish Research Agency, Ministry of Science Technology and Innovation (Dinamarca). 2005-2007. Ib Chorkendorff (UTD). Researcher.
7. *Theoretical study of structural, electronic and thermal properties of nanodimensional systems of technological interest.* Ministerio de Ciencia y Tecnología. 2005-2007. Andrés Vega (UVa). Researcher.



**Part A. PERSONAL INFORMATION**

<b>CV date</b>	31/10/2023
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First name	Silvia Noemí		
Family name	Santalla Arribas		
Gender (*)		Birth date (dd/mm/yyyy)	
Social Security, Passport, ID number			
e-mail	silvia.santalla@uc3m.es		URL Web:
Open Researcher and Contributor ID (ORCID) (*)	00-0002-6521-526X		

(\*) Mandatory

**A.1. Current position**

Position	Associate Professor (Profesor Titular)		
Initial date	16/05/2022		
Institution	Universidad Carlos III de Madrid		
Department/Center	Física	Escuela Politécnica Superior	
Country	Spain	Teleph. number	
Key words	Growth of rugged and biological interfaces. Stochastic geometry. Dynamic structure of surfaces and heterostructures. Molecular dynamics. Entanglement in complex quantum systems.		

**A.2. Previous positions (research activity interruptions, art. 14.2.b))**

Period	Position/Institution/Country/Interruption cause
01/10/00 – 30/09/05	Teaching Assistant (Ayudante de Escuela Universitaria) / Universidad Carlos III de Madrid / Spain
01/10/05 – 06/09/09	Teaching Assistant (Ayudante) / Universidad Carlos III de Madrid / Spain
07/09/09 – 30/09/13	Assistant professor (Profesor Ayudante Doctor) / Universidad Carlos III de Madrid / Spain
01/10/13 – 15/02/22	Assistant professor (Profesor Visitante) / Universidad Carlos III de Madrid / Spain

**A.3. Education**

PhD, Licensed, Graduate	University/Country	Year
Graduate in Physics	Facultad de CC. Físicas, Universidad Complutense de Madrid	15/11/1998
Graduate Thesis	Facultad de CC. Físicas, Universidad Complutense de Madrid	26/06/2001
PhD. Thesis	Facultad de CC. Físicas, Universidad Complutense de Madrid	30/01/2008

**Part B. CV SUMMARY (max. 5000 characters, including spaces)**

My research interests lie at the crossroads between condensed matter and statistical physics, extending from biological growth models to the structure of entanglement in quantum many-body systems. The connecting thread is the characterization of fluctuations and strong correlations in complex systems, both classical and quantum, and the applicability of the notion of universality class. I combine analytical and numerical tools, with a special emphasis on visualization and the insight obtained by interdisciplinary collaborations.

I have developed an academic career based on the Physics Department of Universidad Carlos III de Madrid (UC3M), while establishing research bonds with other institutions, such as the Instituto de Física Teórica (IFT, UAM-CSIC, Madrid), Universidad Nacional de Educación a Distancia (UNED, Madrid), Scuola Internazionale Superiore di Studi Avanzati (SISSA, Trieste) and the Universidade Federal de Viçosa (UFV, Viçosa, Brazil).

My initial research took place at the Departamento de Física Teórica at Universidad Complutense de Madrid (UCM) on the intersection between statistical mechanics and high-energy physics, resulting in one article in Phys. Rev. D and a master thesis (grado de licenciatura) on the non-linear behavior of a pion gas, as it was expected to be observed in large colliders such as LHC at CERN. In 2008 I obtained my Ph.D. applying a variety of mathematical and theoretical tools to the characterization of semiconductor heterostructures under the supervision of Prof. Rosa M. de la Cruz at UC3M while working as a teaching assistant (ayudante), which resulted in the publication of eight articles in indexed journals.

Since 2009 I serve as an assistant professor (prof. ayudante doctor / prof. visitante) at the Physics Department of UC3M, where I have been able to establish my different lines of research. Since that moment I have enjoyed continuous funding from the Spanish Government, as a part of different research teams associated to these lines.

My interest in fractal structures in growing interfaces led to an ongoing collaboration with Prof. Rodolfo Cuerno, at the Mathematics Department of UC3M. Our approach leads to engagement with condensed matter physics experimentalists, such as Prof. Luis Vázquez at ICMM (CSIC), sharing our analytical and numerical tools in order to characterize the observed patterns in the laboratory. Interestingly, the same theoretical tools can be employed in biophysics in order to elucidate the interfaces of growing cell aggregates or bacterial colonies. Following the same approach, we have combined theoretical and experimental work in the same team, with researchers from the Molecular Biology Department at UAM and from the Physics Department of UFV. The power behind the concept of universality is such that we have been able to apply it also to growing structures in social dynamics, where we have considered the dynamics behind the accretion of power and wealth. In all the considered growing structures we have been able to characterize the universality classes in relation to the most relevant underlying mechanisms, providing a very interesting cross-fertilization between statistical mechanics, condensed matter physics and biology. These lines of work have resulted in eight articles in indexed journals.

The characterization of universal dynamics leads to very relevant current mathematical problems, which include random matrix theory, integrability and conformal symmetry. Since 2015, a collaboration with researchers from the Courant Institute led to a research line establishing a link between the dynamics of growing interfaces and the geometry in random manifolds, specially the geodesics and isochrone curves (balls). Again, the concept of universality class comes reinforced, making both theoretical physicists and mathematicians learn together. Currently, I am supervising the Ph.D. work of two students in this line, along with researchers from UNED, developing an application to traffic dynamics. These lines of work have resulted in six articles in indexed journals.

My last line of work is the characterization of the entanglement of quantum complex systems, along with researchers from IFT. It is very interesting to note that the deep mathematical structure behind the universality classes of growing interfaces applies to the dynamics of quantum many-body systems. I have explored these connections in the case of disordered lattices, quantum computation, emergent geometry and the Casimir effect on curved space-times. On this last topic I am supervising a third Ph.D. student, along with researchers from IFT and UNED. These lines of work have resulted in nine articles in indexed journals.

## Part C. RELEVANT MERITS (*sorted by typology*)

### C.1. Publications (see *instructions*)

1. S.N. Santalla, G. Ramírez, S. Singha Roy, G. Sierra, J. Rodríguez-Laguna, *Entanglement links and the quasiparticle picture*, Physical Review B, **107**, L121114 (2023)
2. B. Mula, E.M. Fernández, J. E. Alvarellos, J.J. Fernández, D. García-Aldea, S.N. Santalla, J. Rodríguez-Laguna, *Ergotropy and entanglement in critical spin chains*, Physical Review B, **107**, 075116 (2023)
3. B. Mula, N. Samos Sáenz de Buruaga, G. Sierra, S.N. Santalla, J. Rodríguez-Laguna, *Depletion in fermionic chains with inhomogeneous hoppings*, Physical Review B, **106**, 224204 (2022)
4. E. Rodríguez-Fernández, S.N. Santalla, M. Castro; R. Cuerno, *Anomalous ballistic scaling in the tensionless or inviscid Kardar-Parisi-Zhang equation*, Physical Review E, **106**, 024802 (2022)
5. C. Lajusticia-Costan, S.N. Santalla, J. Rodríguez-Laguna, E. Korutcheva. *Random walkers on a deformable medium*. Journal of Statistical Mechanics: Theory and Experiment, **073207** (2021)
6. B. Mula, S.N. Santalla, J. Rodríguez-Laguna. *Casimir forces on deformed fermionic chains*. Physical Review Research, **3**, 013062 (2021)
7. D. Villarrubia, I. Álvarez Domenech, S.N. Santalla, J. Rodríguez-Laguna and P. Córdoba-Torres. *First-Passage Percolation under extreme disorder: from bond-percolation to Kardar-Parisi-Zhang universality*. Physical Review E, **101**, 062124 (2020)
8. S. Singha Roy, S.N. Santalla, J. Rodríguez-Laguna and G. Sierra. *Entanglement as geometry and flow*. Physical Review B, **101**, 195134 (2020)
9. S.N. Santalla, K. Korutchev, E. Korutcheva and J. Rodríguez-Laguna. *Power accretion in social systems*. Physical Review E, **100**, 012143 (2019)
10. V. Alba, S.N. Santalla, P. Ruggiero, J. Rodríguez-Laguna, P. Calabrese and G. Sierra. *Unusual area-law violation in random inhomogeneous systems*. Journal of Statistical Mechanics: Theory and Experiment, **023105** (2019)

### C.2. Congress

11. S.N. Santalla. *Universal fluctuations of global measurements in planar clusters*. **Poster**. XXIV Congreso de Física Estadística (FisEs'23). Pamplona (España). 25–27/10/2023
12. S.N. Santalla. *Universal fluctuations of global measurements in planar clusters*. **Oral presentation**. StatPhys 28. Tokyo (Japan). 07–11/08/2023.
13. S.N. Santalla. *Geodesics on random surfaces* . **Oral presentation**. StatPhys 27. Buenos Aires (Argentina). 08–12/07/2019.
14. S.N. Santalla. *Nonlocal growth and kinetic roughening in biological systems: bacterial colonies and cell aggregates*. **Poster**. StatPhys 27. Buenos Aires (Argentina). 08–12/07/2019
15. S.N. Santalla. *Entanglement over the rainbow: statistical mechanics of the area law*. **Poster**. StatPhys 27. Buenos Aires (Argentina). 08–12/07/2019
16. S.N. Santalla and S.C. Ferreira. *Non-locality effects in the Eden growth model*. **Poster**. XXI Congreso de Física Estadística (FisEs'17). Sevilla (España). 30/03–01/04/2017
17. S.N. Santalla, J. Rodríguez-Laguna, J.P. Abad, I. Marín, M.M. Espinosa, J. Muñoz-García, L. Vázquez and R. Cuerno. *Fronts of compact bacterial colonies are not in the KPZ universality class*. **Oral presentation**. XX Congreso de Física Estadística (FisEs'15). Badajoz (España). 05–07/10/2015
18. S.N. Santalla, J. Rodríguez-Laguna, T. LaGatta and R. Cuerno. *Random geometry and the KPZ universality class*. **Poster**. Interface fluctuations and KPZ universality class. Kyoto (Japan). 20–23/08/2014
19. S.N. Santalla, J. Rodríguez-Laguna and R. Cuerno. *The role of topology on the Kardar-Parisi-Zhang universality class*. **Oral presentation**. International Conference on Statistical Physics (SigmaPhi2014). Rhodes (Greece). 07–11/07/2014

20. S.N. Santalla, J. Rodríguez-Laguna, T. LaGatta and R. Cuerno. *Random geometry and the KPZ universality class*. **Poster**. International Conference on Statistical Physics (SigmaPhi2014). Rhodes (Greece). 07–11/07/2014

### C.3. Research projects

21. Reference: PID2021-123969NB-I00, AGENCIA ESTATAL DE INVESTIGACION (AEI) (Spain)  
 Title: Emergence of Generic Scale Invariance in Dynamical Complex Systems (MELVILLE)  
 Main researcher: Rodolfo Cuerno Rejado  
 Affiliation Entity: Universidad Carlos III de Madrid  
 Type of participation: Researcher  
 From 01/01/2022 to 31/12/2025
22. Reference: PGC2018-094763-B-I00, MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES (Spain)  
 Title: Simetría y geometría en las fluctuaciones de sistemas espacialmente extensos lejos del equilibrio (Symmetry and geometry in fluctuations of spatially-extended systems far from equilibrium)  
 Main researcher: Rodolfo Cuerno Rejado and Pedro Córdoba Torres  
 Affiliation Entity: Universidad Carlos III de Madrid  
 Type of participation: Researcher  
 From 01/01/2019 to 30/11/2022
23. Reference: P2018/TCS-4342; Programas de Actividades de I+D entre grupos de investigación de la Comunidad de Madrid en tecnologías 2018 (España)  
 Title: Quantum Information Technologies Madrid  
 Main researcher: Miguel Angel Martín-Delgado Alcántara; Luis Alberto Ibort Latre; Juan José García Ripoll; David Pérez García; Vicente Martín Ayuso; Germán Sierra Rodero; Dolores del Campo Maldonado  
 From 01/2019 to 12/2022  
 Type of participation: Researcher
24. Reference: Conselho Nacional de Desenvolvimento Científico e Tecnológico (Brasil)  
 Title: Processos com muitos agentes interagentes em redes complexas e regulares  
 Main researcher: Silvio C. Ferreira  
 From 01/2019 to 12/2021  
 Type of participation: Researcher
25. Reference: FIS2015-66020-C2-1-P, MINISTERIO DE ECONOMIA, INDUSTRIA Y COMPETITIVIDAD (Spain), 23 716.00€.  
 Title: Auto-organización y fluctuaciones en frentes de crecimiento, erosión y delaminado: teoría y simulación (Self-organization and fluctuations in growth, erosion, and dewetting fronts)  
 Main researcher: Rodolfo Cuerno Rejado  
 Affiliation Entity: Universidad Carlos III de Madrid  
 Type of participation: Researcher  
 From 01/01/2016 to 31/12/2018
26. Reference: FIS2012-38866-C05-01, MINISTERIO DE ECONOMIA, INDUSTRIA COMPETITIVIDAD (Spain), 35 100.00€  
 Title: Modelización y simulación de dinámica interfacial de materia dura y blanda (Modeling and simulation of interface dynamics in hard and soft matter)  
 Main researcher: Rodolfo Cuerno Rejado  
 Affiliation Entity: Universidad Carlos III de Madrid  
 Type of participation: Researcher  
 From 01/01/2013 to 30/09/2016

### C.4. Contracts, technological or transfer merits

## **CURRICULUM ABREVIADO (CVA)**

**Fecha:** 15.10.2023

### **Parte A. DATOS PERSONALES**

Nombre y apellidos	Pablo García González		
DNI:			
Número identificación del investigador			

#### **A.1 Situación profesional actual**

Organismo	Universidad Autónoma de Madrid (UAM)		
Dpto./Centro	Departamento Física Teórica de la Materia Condensada Facultad de Ciencias		
Dirección	C/ Francisco Tomás y Valiente 7, 28049 Madrid, Spain		
Teléfono		E-mail	
Categoría profesional	Profesor Titular	Fecha inicio	19.03.2011
Esp. Cód. UNESCO	221110, 221124		
Palabras clave	Estructura electrónica. Teoría de muchos cuerpos. Excitaciones colectivas y de cuasipartícula. Nanoplasmónica		

#### **A.2 Formación académica (título, institución, fecha)**

Licenciatura/Grado/Doctorado	Universidad	Año
Licenciatura	Universidad Complutense de Madrid	1991
Doctorado	Universidad Nacional de Educación a Distancia (UNED)	1997

#### **A.3 Indicadores generales de calidad de la producción científica**

#### **SEXENIOS DE INVESTIGACIÓN**

Número de sexenios: 4 (1995-2000, 2001-2006, 2007-2012, 2013-2018)

Último sexenio reconocido: 2018

#### **PUBLICACIONES**

35 publicaciones (WOS)

Citas totales 1319 (WOS)

10 artículos con más de 50 citas

Promedio citas por artículo: 38.8

Índice h: 20

### **Parte B. RESUMEN LIBRE DEL CURRICULUM**

Pablo García González es Profesor Titular en el Departamento de Física Teórica de la Materia Condensada de la Universidad Autónoma de Madrid desde 2011. Se doctora en julio de 1997 en la Universidad Nacional de Educación a Distancia con la tesis “Desarrollo y aplicación de funcionales de la densidad no locales para sistemas

*no homogéneos de electrones*" bajo la dirección de los Prof. José Enrique Alvarellos (UNED) y Enrique Chacón (ICMM/CSIC), tesis por la que obtuvo premio extraordinario. Durante la tesis efectúa estancias de investigación en la Universidad de La Laguna y en el Centro de Investigación de Jülich. La investigación realizada se centra en el desarrollo de nuevas técnicas para el cálculo de energías totales dentro del formalismo del funcional de la densidad y el estudio de excitaciones colectivas (plasmones) en superficies de plata.

A continuación, realiza una estancia post-doctoral, con una beca del Ministerio de Educación y Ciencia, en el grupo del Prof. Rex W. Godby de la Universidad de York (Reino Unido) realizando investigaciones teóricas dentro de la teoría de muchos cuerpos y desarrollando técnicas novedosas de su aplicación.

Tras su estancia post-doctoral vuelve a España con un contrato de reincorporación de la UNED y, acto seguido, obtiene un contrato de Investigador Ramón y Cajal. Durante ese periodo continua y amplía la línea de investigación abierta en su periodo postdoctoral y colabora activamente con diferentes grupos de investigación europeos, fundamentalmente de la *European Theoretical Spectroscopy Facility*, de la que llega a ser vice-coordinador. Finalizado el contrato Ramón y Cajal obtiene una posición de Profesor Contratado Doctor en la UNED. Durante ese periodo dirige una tesis doctoral y es investigador principal de dos proyectos nacionales y de uno local.

En marzo de 2011 se incorpora al Departamento de Física Teórica de la Materia Condensada como Profesor Titular, focalizando su investigación al estudio teórico de fenómenos en nanoplasmónica, combinando técnicas clásicas como mecano-cuánticas. En ese periodo dirige dos tesis doctorales y es investigador principal de un proyecto nacional.

Además, cuenta con una amplia experiencia docente, ha sido coautor de tres libros de texto, y es Secretario Académico del Departamento de Física Teórica de la Materia Condensada desde 2014.

## Parte C. MÉRITOS MÁS RELEVANTES

### C.1. Publicaciones recientes

1. *Visualizing screening in noble-metal clusters: static vs. dynamic*  
Sinha-Roy, R., García-González, P., López-Lozano, X., Weissker, H.-C.  
Physical Chemistry Chemical Physics 25, 2075-2083 (2022)

2. *Direct Visualization and Effects of Atom-Scale Defects on the Optoelectronic Properties of Hexagonal Boron Nitride*  
Ares, P., Santos, H., Lazic, S., Gibaja, C., Torres, I., Pinilla, S., Gómez-Herrero, J., van der Meulen, H. P., García-González, P., Zamora, F.  
Advanced Electronic Materials 7, 2001177 (2021)  
Citadas: 8

3. *How metallic are noble-metal clusters? Static screening and polarizability in quantum-sized silver and gold nanoparticles*

Sinha-Roy, R., García-González, Weissker, H.-C.

Nanoscale 12, 4452-4458 (2020)

Citas: 7

4. *Identifying Electronic Modes by Fourier Transform from  $\delta$ -Kick Time-Evolution TDDFT Calculations*

Sinha-Roy, R., García-González, P., López-Lozano, X., Whetten, R., Weissker, H.-C.

Journal of Chemical Theory and Computation 14, 6417-6426 (2018)

Citas: 15

5. *Classical and ab Initio Plasmonics Meet at Sub-nanometric Noble Metal Rods*

Sinha-Roy, R., García-González, P., Weissker, H.-C., Rabilloud, F., Fernández-Domínguez A.I.

ACS Photonics 4, 1484-1493 (2017)

Citas: 49

6. *In Search of the Quantum-Electronic Origin of Color Change: Elucidation of the Subtle Effects of Alloying with Copper on 1.8 nm Gold Nanoclusters*

Sinha-Roy, R., López-Lozano, X., Whetten, R., García-González, P., Weissker, H.-C.

Journal of Physical Chemistry C 121, 5753-5760 (2017)

Citas: 9

7. *Quantum plasmonics: from jellium models to ab initio calculations*

Varas, A., García-González, P., Feist, J., García-Vidal, F.J., Rubio, A.

Nanophotonics 5, 409-426 (2016)

Citas: 103

8. *Stability of the Dirac cone in artificial graphene formed in quantum wells: A computational many-electron study*

Kylanpa, I., Berardi, F., Rasanen, E., García-González, P., Rozzi, C., Rubio, A.

New Journal of Physics 18, 083014 (2016)

Citas: 5

9. *Anisotropy Effects on the Plasmonic Response of Nanoparticle Dimers*

Varas, A., García-González, J., García-Vidal, F.J., Rubio, A.

Journal of Physical Chemistry Letters 6, 1891-1898 (2015)

Citas: 30

10. *Ab initio nanoplasmonics: The impact of atomic structure*

Zhang, P., Feist, J., Rubio, A., García-González, J., García-Vidal, F.J.

Physical Review B 90, 161407 (2014)

Citas: 134

## C.2 Proyectos de investigación

### Investigador principal:

<b>TÍTULO DEL PROYECTO:</b>	Mecánica Estadística de Fluidos Clásicos y Cuánticos	
<b>ENTIDAD FINANCIADORA:</b>	DGI (ref. FIS2004-05035-C03-03)	
<b>DURACIÓN</b>	DESDE: 2004	HASTA: 2007
<b>TÍTULO DEL PROYECTO:</b>	Aplicaciones en la frontera de la espectroscopía teórica: Nanoestructuras y sistemas complejos	
<b>ENTIDAD FINANCIADORA:</b>	DGI (ref. FIS2007-65702-C02-02)	
<b>DURACIÓN</b>	DESDE: 2007	HASTA: 2010
<b>TÍTULO DEL PROYECTO:</b>	Estudio de la dinámica de sistemas cuánticos complejos: Desde desarrollos teóricos fundamentales a aplicaciones energéticas	
<b>ENTIDAD FINANCIADORA:</b>	DGI (ref. FIS2010-21282-C02-02)	
<b>DURACIÓN</b>	DESDE: 2011	HASTA: 2014

### Participante:

12 proyectos nacionales y dos europeos

## C.3 Otros méritos

### Participación en congresos

Organizador de cuatro congresos internacionales

Ponente invitado en diez congresos internacionales

~ 100 contribuciones orales y posters en congresos nacionales e internacionales

### Premios y ayudas recibos

Beca predoctoral FPU del Ministerio de Educación y Ciencia (1993-1996)

Premio extraordinario de doctorado

Beca postdoctoral del Ministerio de Educación y Cultura (1998-2000)

Contrato de investigación Ramón y Cajal (2004-2009)

### Tesis doctorales dirigidas

Jeil Jung Woo (UNED, 2005): *Estudio de la correlación electrónica en sistemas inhomogéneos simples*

Alejandro Varas Barbosa (UPV, 2017): *Modelling linear and non-linear light-matter interactions: From classical to atomistic nanoplasmonics*

Rajarshi Sinha-Roy (UAM / Université Aix-Marseille, 2018): *Ab-initio simulations of optical properties of noble-metal clusters*

### Revisión de artículos y proyectos

Revisor habitual de diferentes revistas internacionales (Science, Physical Review Letters, Physical Review, Journal of Chemical Physics, PCCP, etc.)  
Revisor de proyectos nacionales e internacionales (NFS, FONCYT)

## CURRICULUM VITAE ABREVIADO (CVA)

**IMPORTANT** – *The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.*

### Part A. PERSONAL INFORMATION

First name	Javier		
Family name	Rodríguez-Laguna		
Gender		Birth date (dd/mm/yyyy)	
ID number			
e-mail		Web	
Open Researcher and Contributor ID (ORCID)	0000-0003-2218-7980		

#### A.1. Current position

Position	Full Professor (Catedrático de Universidad)		
Initial date	July 12, 2023		
Institution	Universidad Nacional de Educación a Distancia (UNED)		
Department/Center	Fundamental Physics		
Country	Spain	Phone	
Key words	Condensed matter physics, quantum many-body systems, entanglement, statistical mechanics, quantum technologies		

#### A.2. Previous positions (research activity interruptions, indicate total months)

Period	Position/Institution/Country/Interruption cause		
1996-2005	Secondary school teacher, Madrid, Spain (9 years)		
2005-07	Postdoctoral researcher, SISSA, Italy (2 years)		
2007-11 & 2013-14	Assistant professor (ayudante doctor), UC3M, Spain (5 years)		
2011-12	Researcher, ICFO, Spain (18 months)		
2012-13	Researcher, IEM (CSIC), Spain (7 months)		
2013	Researcher, ICMAT (CSIC-UC3M), Spain (3 months)		
2015-20	Researcher, UNED, Spain (5 years)		
2020-23	Associate Professor, UNED, Spain (3.5 years)		

#### A.3. Education

Degree	University/Country	Year
Ph.D. in Theoretical Physics	Universidad Complutense de Madrid, Spain	2002
Graduate in Physics / Licenciado	Universidad Complutense de Madrid, Spain	1995

#### Part B. CV SUMMARY (max. 5000 characters, including spaces)

- 70 JCR articles (most in Q1). Citations: 1222 (Scholar), 827 (WoS).
- Six Ph.D. thesis supervised, 2014-2023: 1 at ICFO, 3 at IFT (UAM-CSIC), 2 at UNED.
- PI of a current national project (along with Eva M. Fernández).

**Trajectory.** After my graduation in Physics from UCM (1995) I worked as a secondary school teacher of mathematics at public schools in Madrid for nine years (1996-2005). In the meantime I defended my Ph.D. thesis on the renormalization group, combining analytical and numerical approaches, such as conformal field theory and the DMRG, under the supervision of Professors Germán Sierra and Miguel Ángel Martín-Delgado (IMAFF-CSIC and UCM), which received the *premio extraordinario de doctorado*. From 2005 to 2007 I was a postdoc researcher at SISSA (Trieste, Italy). In 2007 I returned to Madrid as an assistant professor at Universidad Carlos III de Madrid, in the Mathematics Dept. (2007-11 and 2013-14), where I worked in the group of Prof. Rodolfo Cuerno. In 2011-12 I joined the group of Prof. Maciej Lewenstein at ICFO (Barcelona), followed by research periods at IEM-CSIC (2012-13) and ICMAT (2013). Since 2014, I am also a visiting researcher at IFT (UAM-CSIC), in the group



of Prof. Germán Sierra. In Jan. 2015 I entered the Fundamental Physics Dep. at UNED as a researcher, where I was allowed to develop my own research lines. In 2019 I received an I3 certificate for outstanding research, and one year later I obtained a permanent position in the same department. In July 2023 my position was upgraded to full professorship.

**Research lines.** My research scope is very broad within the fields of statistical mechanics and quantum many-body systems, with applications ranging from quantum technologies or quantum thermodynamics to stochastic geometry or epidemic spread. The main thread along my work is methodological: I am interested in entanglement, strong correlations and fluctuations, specially their interplay with geometry, structure and disorder. I apply both theoretical tools (e.g. conformal field theory) and computational tools (e.g. density matrix renormalization group, Monte Carlo, etc.), with a strong emphasis on visualization.

**Scientific publications.** I have published 70 articles in JCR journals, most of them Q1, yielding an h-index 17 and over 1200 citations (Scholar). My articles include 2 Phys. Rev. Lett., 4 New J. Phys., 1 Nano Lett., and two single-authored papers. More than half of my scientific production was published during my current stage at UNED (42 JCR articles since 2015). Among my most relevant contributions I would like to remark the development of the *rainbow system*, a quantum chain whose ground state presents maximal entanglement between symmetrically placed sites, the characterization of the interplay between entanglement and disorder, the design of quantum simulators to probe the Unruh-Hawking effect, and the realization that geodesics and balls in 2D stochastic manifolds are fractals following Kardar-Parisi-Zhang universality. All these results were developed along with researchers from different institutions, some of them foreign (SISSA, UC3M, ICFO, IFT and Courant Institute).

**Other contributions.** I have supervised six Ph.D. thesis (1 at ICFO, in 2014; 3 at IFT, in 2015, 2018 and 2022; 2 at UNED in 2023), and two more are in progress, and contributed to the consolidation of the Statistical Mechanics of Complex Systems group at UNED, bringing together researchers with different backgrounds. Currently, I am PI of a Spanish national research project, along with Prof. Eva M. Fernández, and I have been member of other 6 national projects and one from *Comunidad de Madrid*. I contribute to the *open science* movement by publishing all my research in ArXiv and submitting my research code to open repositories, such as github. Also, I am interested in scientific outreach, creating videos at the IFT youtube channel, giving talks at Ateneo de Madrid and publishing articles in The Conversation.

## Part C. RELEVANT MERITS (sorted by typology)

### C.1. Publications (see instructions)

[Ergotropy and entanglement in critical spin chains](#), B. Mula, E.M. Fernández, J.E. Alvarellos, J.J. Fernández, D. García-Aldea, S.N. Santalla and JRL, Phys. Rev. B **107**, 075116 (2023).

[Casimir forces on deformed fermionic chains](#), B. Mula, S.N. Santalla, JRL, Phys. Rev. Research **3**, 013062 (2021). Characterizes the Casimir forces for the Dirac vacuum on curved spacetimes, along with a proposal for a quantum simulator. 10 citations.

[Entanglement as geometry and flow](#), S. Singha Roy, S.N. Santalla, JRL, G. Sierra, Phys. Rev. B **101**, 195134 (2020). Introduces the entanglement links, which describe the emergent geometry behind a certain entanglement structure. 13 citations.

[Entanglement Hamiltonian and entanglement contour in inhomogeneous 1D systems](#), E. Tonni, JRL, G. Sierra, JSTAT 043105 (2018). Shows a relation between the entanglement Hamiltonian and contour, applying it to the Dirac vacuum on curved spacetimes. Collaboration with SISSA (Italy). 82 citations.

[More on the rainbow chain: entanglement, space-time geometry and thermal states](#), JRL, J. Dubail, G. Ramirez, P. Calabrese, G. Sierra, J. Phys. A **50**, 164001 (2017). Shows that the

rainbow system can be explained as a spin chain on a curved spacetime. Collaboration with SISSA (Italy) and CNRS (France). 40 citations.

Synthetic Unruh effect in cold atoms, JRL, L. Tarruell, M. Lewenstein, A. Celi, Phys. Rev. A **95**, 013627 (2017). Proposes a quantum simulator for the Unruh effect able to show the expected statistics inversion (Bose/Fermi) depending on the space dimension. Collaboration with ICFO (Barcelona). 65 citations.

Entanglement in correlated random spin chains, RNA folding and kinetic roughening, JRL, S.N. Santalla, G. Ramírez, G. Sierra, New J. Phys. **18**, 073025 (2016). Describes long-range entanglement in certain random spin chains with correlated couplings, employing an analogy with RNA folding and kinetic roughening. 22 citations.

Random geometry and the Kardar-Parisi-Zhang universality class, S.N. Santalla, J. Rodríguez-Laguna, T. LaGatta, R. Cuerno, New J. Phys. **17**, 033018 (2015). Characterizes the fractal properties of geodesics in random manifolds using the KPZ class. Collaboration with Courant Institute (USA). 19 citations.

From conformal to volume-law for the entanglement entropy in exponentially deformed critical chains, G. Ramírez, JRL, G. Sierra, JSTAT P10004 (2014). Introduces the rainbow chain, whose ground state shows maximal entanglement. 67 citations.

H=xp model revisited and the Riemann zeros, G. Sierra, JRL, Phys. Rev. Lett. **106**, 200201 (2011). Analysis of Hamiltonians whose spectrum resembles the imaginary parts of the non-trivial zeros of the Riemann zeta function. 77 citations.

Anderson transition in low-dimensional disordered systems driven by long-range nonrandom hopping, A. Rodríguez, V.A. Malyshev, G. Sierra, M.A. Martín-Delgado, JRL, F. Domínguez-Adame, Phys. Rev. Lett. **90**, 027404 (2003). Explores the limits of Anderson's theorem on localization by disorder with long range correlations. 131 citations.

**C.2. Conferences**, indicating the modality of their participation (invited conference, oral presentation, poster)

Oral presentation, *Entanglement over the rainbows*, StatPhys'28, Tokyo (Japan), Aug. 2023.

Oral presentation, *Topology and the KPZ universality class*, Interface Fluctuations and KPZ Universality Class, Yukawa Institute of Theoretical Physics, Kyoto (Japan), August 2014.

Oral presentation, *Simulated disorder entails perfect discipline*, Quantum Integrability, Conformal Field Theory and Topological Quantum Computation, International Institute of Physics (IIP), Natal (Brazil), March 2014.

Oral presentation, *Simulating the Unruh effect in artificial Rindler spacetime*, Relativistic Quantum Information meets Analogue Gravity, Nottingham (UK), March 2013.

Oral presentation, *Simulating quantum matter near event horizons*, Quantum Simulators, Bilbao (Spain), October 2012.

Oral presentation, *Quantum optimization: spin glasses and wavefunction annealing*, American Physical Society (APS) March Meeting, Denver (USA), March 2007.

Oral presentation, *DMRG applied to diagonal ladders*, and poster, *Real space RG methods for quantum mechanics in >1D*, Density Matrix Renormalization workshop, Lorentz Center, Leiden (Netherlands), Aug. 2004.

**C.3. Research projects**, indicating your personal contribution.

*Quantum complex systems: fundamentals and applications*, COSY-QUEST, PID2019-105182GB-I00, Spanish Gov. PI: Eva M. Fernández and Javier Rodríguez-Laguna (UNED). Since June 2020.

*Quantum information technologies Madrid*, QUITEMAD-CM, P2018-TCS434, Madrid local Gov. PI: Miguel Ángel Martín-Delgado (UCM). Jan. 2019 to Dec 2021.

*Quantum entanglement in quantum many particle systems*, FIS2015-69167-C2-1, Spanish Gov. PI: Germán Sierra. Jan. 2016 to Dec. 2018.

*Modelling and simulation of interface dynamics in hard and soft matter systems*, FIS2012-38866-C05-01, Spanish Gov. PI: Rodolfo Cuerno (UC3M). Jan. 2013 to Dec. 2015.

*Topological quantum matter: in the boundary between condensed matter, quantum optics and quantum information*, FIS2012-33642, Spanish Gov. PI: Belén Paredes (UAM-CSIC). Jan. 2013 to Dec. 2015.

*Theoretical physics of condensed matter and quantum information*, FIS2009-11654, Spanish Gov. PI: Germán Sierra (UAM-CSIC). Jan. 2010 to Dec. 2012.

*Theoretical approaches to the dynamics and fluctuations of (sub)microscopic interfaces*, FIS2009-12964-C05-01, Spanish Gov. PI: Rodolfo Cuerno (UC3M). Jan. 2010 to Dec. 2012.

*Analytical and exact numerical methods in condensed matter*, FIS2006-04885, Spanish Gov. PI: Germán Sierra (UAM-CSIC). Jan. 2007 to Dec. 2009.

#### **C.4. Contracts, technological or transfer merits.**

CV Date	05/10/2022
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## Part A. PERSONAL INFORMATION

First Name *	Miguel Angel		
Family Name *	Rubio Alvarez		
Sex *		Date of Birth *	
ID number Social Security, Passport *		Phone Number *	(+34) 913987129
URL Web			
Email Address	mar@fisfun.uned.es		
Researcher's identification number	Open Researcher and Contributor ID (ORCID) *	0000-0002-4210-0443	
	Researcher ID	A-4093-2008	
	Scopus Author ID	57200105177	

\* Mandatory

### A.1. Current position

Job Title	Catedrático de Universidad		
Starting date	1996		
Institution	Universidad Nacional de Educación a Distancia		
Department / Centre	Física Fundamental / Facultad de Ciencias		
Country	Spain	Phone Number	913987129
Keywords	Monolayers; Rheology; Colloids; Polymers; Complex fluids		

### A.2. Previous positions

Period	Job Title / Name of Employer / Country
2016 -	Director del Departamento de Física Fundamental / Universidad Nacional de Educación a Distancia

### A.3. Education

Degree/Master/PhD	University / Country	Year
Doctor en Ciencias Físicas	Universidad Nacional de Educación a Distancia	1985
Licenciado en Ciencias Físicas, con Grado	Universidad Complutense de Madrid	1979

### A.4. General quality indicators of scientific production

Sexenios de investigación: 6 (todos los posibles). Último concedido: 2012-2017.

Tesis dirigidas en los últimos 10 años: 2 de un total de 8. Cuatro de ellas obtuvieron Premio Extraordinario de Doctorado. Entre julio del 2009 y julio del 2013 fui Vicerrector de Profesorado y Vicerrector 1º y decidí no dirigir Tesis Doctorales durante dicho periodo.

Número total de artículos publicados en revistas: 71; 50 (70%) en el primer cuartil (Q1).

Factor h: 24 (Google Scholar); 22 (Publons)

Número de citas totales: 2.804 (Google Scholar); 1.926 (Publons).

Número medio de citas por artículo: 39,5 (Google Scholar); 27,13 (Publons)

Promedio de citas por año en los últimos 5 años: 129,8 (Google Scholar); 91,6 (Publons).

## Part B. CV SUMMARY

I started my doctorate studies at the end of 1981 under the supervision of Prof. Manuel G. Velarde. In the pre-doctoral period I carried out experimental research stays at CEA (Saclay, France, 6 months in total; supervised by Dr. Pierre Bergé and Dr. Monique Dubois) and at the Istituto Nazionale di Ottica (Florence, Italy, 16 months in total; supervised by Prof. F.Tito Arecchi

and Dr. Sergio Ciliberto). I obtained a PhD in Physics in 1985 from UNED and a permanent position as Adjoint Professor at UNED in 1988. At that time my research focused on nonlinear dynamics in different physical systems (Rayleigh-Bénard and Bénard-Marangoni convection, Helmholtz oscillator, etc.) and I published several scientific articles with wide repercussion. Notably, two in Phys Rev. Lett., with 181 and 166 citations (Publons index). From November 1988 to January 1990, I enjoyed a research stay at Prof. Jerry P. Gollub's lab (Haverford College, USA), funded by a senior fellowship from the Scientific Office of NATO, during which I worked on the structure of fluid interfaces in porous media imbibition as model systems for surface growth with quenched noise, also with wide repercussion (Phys. Rev. Lett., with 278 citations).

Overall, I have published 68 articles in highly recognized scientific journals such as Phys. Rev. Lett. (7), Phys. Rev. E (9), Appl. Phys. Lett. (3), J. of Rheology (3), J. Colloid Interf. Sci. (3), Adv. Coll. Interf. Sci (1), Current Opinion in Coll. Interf. Sci. (1), etc., which have obtained 1746 citations according to Publons index (2498 according to Google Scholar).

At the beginning of 1990 I started the activities of the Complex Systems Laboratory at UNED. Since then my interests have focused on experimental Soft Matter Physics (colloids, polymers, interfaces, etc.). In 1996 I obtained a position as University Professor at UNED, working in the Applied Physics area. Between 1996 and 2009 my research focused on magnetic colloids, collaborating with GG Fuller (U. Stanford, USA) and A.A. García (U. Arizona State, USA). We obtained relevant results on the aggregation kinetics of superparamagnetic particles in suspension under stationary and rotating magnetic fields and on the use of magnetic particles in the microfluidics of drops standing on superhydrophobic surfaces. In July 2009 I was appointed Vice-Rector for Teaching Staff of the UNED and, in September 2010, First Vice-Rector, positions that slowed down my research activity during the four years in office (until July 15, 2013). Subsequently, I started a new line of research focused on the mechanical properties of Langmuir monolayers, where we have achieved significant improvements in the magnetic needle interfacial shear rheometer, using magnetic microwire probes and magnetic tweezers to control their movement. The results are impressive gains in the instrument's resolution (a 1000 factor) and in the stability of the sample-probe system, that lead to a granted european patent whose licensing is being negotiated with Biolin Scientific. Furthermore, we have extended with great success the flow field-based data analysis techniques to the case of rotational rheometers with different probes. At present my main research interests are: i) the development of new interfacial rheology techniques, both shear and dilatational, and ii) the interfacial rheology of monomolecular films of soft matter systems (fatty acids, insoluble polymers, proteins, lipids of biomedical interest, biofilms, etc.).

## Part C. RELEVANT ACCOMPLISHMENTS

### C.1. Publications

AC: corresponding author. (nº x / nº y): position / total authors. If applicable, indicate the number of citations

- 1 **Scientific paper.** P. Domínguez; M. Pancorbo; F. Ortega; M.A. Rubio. 2018. JColloids: Image analysis for video-microscopy studies of colloidal suspensions Computer Physics Communications. Elsevier. 231, pp.243-244. <https://doi.org/10.1016/j.cpc.2018.04.033>
- 2 **Scientific paper.** P. Sánchez-Puga; J. Tajuelo; J.M. Pastor; M.A. Rubio. 2021. BiconeDrag updated-A data processing application for the oscillating conical bob interfacial shear rheometer Computer Physics Communications. North-Holland. 267, pp.108074.
- 3 **Scientific paper.** P. Sánchez-Puga; J. Tajuelo; J.M. Pastor; M.A. Rubio. 2021. Dynamic Measurements with the Bicone Interfacial Shear Rheometer: The Effects of the Numerical Implementation of the Interfacial Boundary Condition Colloids and Interfaces. MDPI. 5-1, pp.1-17.
- 4 **Scientific paper.** Pablo Sánchez Puga; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz; Miguel Ángel Rubio Álvarez. 2020. Flow field-based data analysis in interfacial shear rheometry Advances in Colloid and Interface Science. Elsevier. <https://doi.org/10.1016/j.cis.2020.102332>

- 5 **Scientific paper.** Óscar Toledo; Miguel Ángel Rubio Álvarez; Óscar Gálvez. 2020. Energetics and structures of the tilted phases of fatty acid Langmuir monolayers Phys. Chem. Chem. Phys. Royal Society of Chemistry. 22, pp.12092-12103. <https://doi.org/10.1039/D0CP01361G>
- 6 **Scientific paper.** Pablo Sánchez-Puga; Javier Tajuelo; Juanma Pastor; M.A. Rubio. 2019. BiconeDrag—A data processing application for the oscillating conical bob interfacial shear rheometer Computer Physics Communications. Elsevier. 239, pp.184-196.
- 7 **Scientific paper.** Pablo Sánchez-Puga; Javier Tajuelo; Juanma Pastor; M.A. Rubio. 2018. Dynamic Measurements with the Bicone Interfacial Shear Rheometer: Numerical Bench-Marking of Flow Field-Based Data Processing Colloids and Interfaces. MDPI. 2-4, pp.69-87.
- 8 **Scientific paper.** E. Guzmán; J. Tajuelo; J.M. Pastor; M.A. Rubio; F. Ortega; R.G. Rubio. 2018. Shear rheology of fluid interfaces: Closing the gap between macro- and micro-rheology Current Opinion in Colloid & Interface Science. Elsevier. 37, pp.33-48. <https://doi.org/10.1016/j.cocis.2018.05.004>
- 9 **Scientific paper.** F. Martínez-Pedrero; J. Tajuelo; P. Sánchez-Puga; R. Chuliá-Jordán; F. Ortega; M.A. Rubio; R.G. Rubio. 2018. Linear shear rheology of aging ?-casein films adsorbing at the air/water interface Journal of Colloid and Interface Science. Elsevier. 511, pp.12-20. <https://doi.org/10.1016/j.jcis.2017.09.092>
- 10 **Scientific paper.** J. Tajuelo; J.M. Pastor; M.A. Rubio. 2017. Flow field based data processing for the oscillating conical bob interfacial shear rheometer Journal of Rheology. The Society of Rheology. 62-1, pp.295-312. <https://doi.org/10.1122/1.5012764>
- 11 **Scientific paper.** J. Tajuelo; E. Guzmán; F. Ortega; R.G. Rubio; M. A. Rubio. 2017. Phase diagram of fatty acid Langmuir monolayers from rheological measurements Langmuir. American Chemical Society. 33, pp.4280-4290. <https://doi.org/DOI:10.1021/acs.langmuir.7b00613>

## C.2. Conferences and meetings

- 1 Pablo Sánchez Puga; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz; Miguel Ángel Rubio Álvarez. Nonlinear interfacial strain profiles in the magnetic needle ISR and the constant strain operation modes. Annual European Rheology Conference. European Society of Rheology. 2022. Spain. Conference.
- 2 Miguel Ángel Rubio Álvarez; Pablo Sánchez Puga; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz. Two-dimensional melting in untilted phases of fatty acid Langmuir monolayers: a thermo-rheological study. Liquid Matter Conference. European Physical Society. 2021. Conference.
- 3 Pablo Sánchez Puga; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz; Miguel Ángel Rubio Álvarez. Flow field-based data analysis for rotating microfabricated probes (the microbutton ISR). Annual European Rheology Conference. European Society of Rheology. 2021. Conference.
- 4 Pablo Sánchez Puga; Javier Tajuelo Rodríguez; Miguel Ángel Rubio Álvarez. Phase transitions in fatty acid Langmuir monolayers: a thermo-rheological study of the transitions to the LS phase. 10th International Colloids Conference. Elsevier. 2020. Spain. 'Participatory - poster. Conference.
- 5 Pablo Sánchez Puga; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz; Miguel Ángel Rubio Álvarez. Thermo-rheological studies of phase transitions in fatty acid Langmuir monolayers: Transitions to the LS phase. 18th International Congress on Rheology. 2020. Brazil. Participatory - oral communication. Conference.
- 6 Miguel Ángel Rubio Álvarez; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz; Pablo Sánchez Puga. Dynamic measurements with the bicone interfacial shear rheometer: Flow field based data processing.. 16th Conference of the International Association of Colloid and Interface Scientists. International Association of Colloid and Interface Scientists. 2018. Holland. Participatory - oral communication. Conference.

- 7 Fernando Martínez Pedrero; Javier Tajuelo Rodríguez; Pablo Sánchez Puga; Francisco Ortega; Miguel Ángel Rubio Álvarez; Ramón González Rubio. Linear shear rheology of aging B-casein films adsorbing at the air/water interface. 12th Annual European Rheology Conference. The European Society of Rheology. 2018. Italy. Participatory - oral communication. Conference.
- 8 Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz; Miguel Ángel Rubio Álvarez. The bicone interfacial shear rheometer revisited: Flow field based data processing for the oscillating conical bob. 12th Annual European Rheology Conference. The European Society of Rheology. 2018. Italy. Participatory - oral communication. Conference.
- 9 Javier Tajuelo Rodríguez; Eduardo Guzmán; Ramón González Rubio; Francisco Ortega; Miguel Ángel Rubio Álvarez. Phase transitions in fatty acid Langmuir monolayers: Interfacial shear rheology results. VII Iberian Meeting on Colloids and Interfaces. 2017. Spain. Participatory - oral communication. Conference.
- 10 Javier Tajuelo Rodríguez; Eduardo Guzmán; Francisco Ortega; Ramón González Rubio; Miguel Ángel Rubio Álvarez. The unusual interfacial shear rheology of fatty acid/alcohol Langmuir monolayers. 11th Annual European Rheology Conference. European Society of Rheology. 2017. Denmark. Participatory - oral communication. Conference.

#### C.3. Research projects and contracts

- 1 **Project.** Teoría del Coarse-Graining y técnicas experimentales para sistemas biológicos multiescala. Ministerio de Ciencia e Innovación. Pep Español Garrigós. (Universidad Nacional de Educación a Distancia). 01/09/2021-31/08/2024. 145.200 €.
- 2 **Project.** Estructura y Dinámica Multiescala en Materia Blanda. Ministerio de Ciencia e Innovación. Investigación. José Español Garrigós. (Universidad Nacional de Educación a Distancia). 01/01/2017-31/12/2019. 54.450 €.
- 3 **Project.** Reología interfacial y estabilidad de películas delgadas fluidas. Ministerio de Ciencia e Innovación. Investigación. Miguel Ángel Rubio Álvarez. (Universidad Nacional de Educación a Distancia). 01/10/2017-30/09/2018. 10.000 €.
- 4 **Contract.** Collaboration agreement by and between UNED and Biolin Scientific Miguel Ángel Rubio Álvarez. 15/02/2021-15/02/2036.

#### C.4. Activities of technology / knowledge transfer and results exploitation

- 1 Miguel Ángel Rubio Álvarez; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz. 16829899.0 - 1001 / 3330695. Magnetic needle interfacial shear rheometer and system and method for actuating same 09/09/2020. Universidad Nacional de Educación a Distancia.
- 2 Miguel Ángel Rubio Álvarez; Javier Tajuelo Rodríguez; Juan Manuel Pastor Ruiz. P201531113. Reómetro interfacial de cizalla por aguja magnética y sistema y método de accionamiento del mismo Spain. 01/12/2017. Universidad Nacional de Educación a Distancia, Universidad Politécnica de Madrid.
- 3 Miguel Ángel Rubio Álvarez; Javier Tajuelo Rodríguez; Fernando Martínez Pedrero; Ramón González Rubio; Francisco Ortega Gómez; Juan Manuel Pastor Ruiz. P201431106. Procedimiento de calibración para sondas magnéticas de reómetros interfaciales de cizalla por aguja magnética Spain. 26/05/2015. Universidad Nacional de Educación a Distancia, Universidad Complutense, Universidad Politécnica de Madrid.

## CURRICULUM VITAE ABREVIADO (CVA)

**IMPORTANT** – The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.

### Part A. PERSONAL INFORMATION

First name	Amalia
Family name	Williart Torres
Gender	

#### A.1. Current position

Position	Profesora Titular de Universidad		
Initial date	21/04/2003		
Institution	Universidad Nacional de Educación a Distancia		
Department/Center	Física Interdisciplinar	Facultad de Ciencias	
Country	Spain	Teleph. number	913987184
Key words	Radiaciones ionizantes. Interacción de la radiación con materiales de interés radiológico y medioambiental		

#### A.2. Previous positions (research activity interruptions, indicate total months)

Period	Position/Institution/Country/Interruption cause
1/05/1990-1/05/1991	Profesora asociada a tiempo parcial/F. de Ciencias/UNED
1/05/1991-1/10/1999	Profesora asociada a tiempo completo/F.de Ciencias/UNED
1/10/1999-2/07/2001	PTEU interina//F. de Ciencias/UNED
1/07/2001-21/04/2003	PTEU /F .de Ciencias/UNED

#### A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Licenciada en Ciencias Físicas	Universidad Complutense de Madrid	1988
Doctora en Ciencias Físicas	Universidad Complutense de Madrid	1996

(Include all the necessary rows)

### Part B. CV SUMMARY

Valoración positiva de dos sexenios de investigación, el último concedido en resolución del 5 de junio de 2019.

Número total de citas: 1149

Promedio de citas: 9,3 citas/año

Publicaciones totales en Q1: 7

Índice h = 8

Participación en los sucesivos proyectos de investigación liderados por el IP Gustavo García Gómez-Tejedor del CSIC, en los que se ha estudiado la interacción de la radiación (electrones secundarios, rayos X, rayos gamma) con sistemas de interés biomédico y su relación con el daño por radiación (véase C2). Esta colaboración se ha llevado a cabo tanto en los locales del CSIC como en los de la UNED. Fruto de esta colaboración han sido varias publicaciones y la presentación de diversos resultados en congresos, tanto nacionales como internacionales.

En el laboratorio de interacción radiación-materia (Unidad Asociada al CSIC durante 11 años) sito en la Facultad de Ciencias de la UNED, cuya investigadora responsable es A. Williart, se ha puesto a punto un sistema experimental de rayos X para el estudio de las

interacciones de electrones secundarios. Montaje de diversos sistemas espectroscópicos para realizar medidas de distintos emisores de radiación ( $\text{I-125}$ ,  $\text{Ru-106}$ , entre otros) y de la interacción de las distintas emisiones (electrones, positrones, gamma) con varios materiales.

También ha realizado labores de gestión de la investigación, en el Comité de Organización de tres congresos celebrados en Madrid.

Además durante 9 años (2005-2014) ha realizado actividades de gestión de la investigación como Vicedecana de Investigación de la Facultad de Ciencias de la UNED.

Y durante 8 años ha sido Directora del Departamento de Física Interdisciplinar (antes de los Materiales) de la UNED (desde noviembre del 2015 hasta octubre del 2023).

Ha participado en numerosas actividades de divulgación científica sobre temas relacionados con el uso de las Radiaciones Ionizantes, Energía e Impacto ambiental de la energía en colaboración con la Real Sociedad Española de Física, entre otros.

### Part C. RELEVANT MERITS (sorted by typology)

#### C.1. Publications

- Autores (p.o. de firma): A. Williart, A. Muñoz, D. Boscolo, E. Scifoni M. Krämer, G. García  
Título: ***Study on Tl-204 simultaneous electron and photon spectra and their interaction with gold absorbers. Experimental results and Monte Carlo simulations.***  
Ref. Nucl. Inst. Meth. Phys. Res. A  
Volumen: 927 pags. 435-442. Fecha: Marzo 2019
- Autores (p.o. de firma): R. Colmenares, A. Williart, A. Muñoz, F. Blanco, G. García and K. Krupa  
Título: ***A process to describe radiation damage at the molecular level. Application to I-125 seeds in water.***  
Ref. Applied radiation and isotopes  
Volumen: 140 pags. 163-170. Fecha: Mayo 2018
- Autores (p.o. de firma): A. Ferrer, M. Shaw y A. Williart  
Título: ***Física Nuclear y de Partículas***  
Fecha: 2013  
Número de páginas: 520  
Editorial: UNED 6104403GR02A01  
Lugar de publicación: Madrid
- Autores (p.o. de firma): M. Shaw y A. Williart  
Título: ***Física Nuclear y de Partículas: Problemas Resueltos***  
Fecha: 2013  
Número de páginas: 262  
Editorial: UNED 6104403GR01A01  
Lugar de publicación: Madrid
- Autores (p.o. de firma): M.C. Fuss, A. Muñoz, J.C. Oller, F. Blanco, A. Williart, P. Limão-Vieira, M.J.G. Borge, O. Tengblad, C. Huerga, M. Téllez and G. García  
Título: ***Energy deposition by a  $^{106}\text{Ru}/^{106}\text{Rh}$  eye applicator simulated using LEPTS, a Low-Energy Particle Track Simulation***  
Ref. Applied Radiation and Isotopes  
Volumen: 69 pags. 1198-1204 Fecha: Abril 2011  
Lugar de publicación: Holland
- Autores (p.o. de firma): M.C. Fuss, A. Muñoz, J.C. Oller, F. Blanco, P. Limão-Vieira, A. Williart, C. Huerga, M. Téllez and G. García  
Título: ***Energy deposition model for I-125 photon radiation in water***  
Ref. Eur. Phys. J. D  
Volumen: 60 pags. 203-208 Fecha: Octubre 2010  
Lugar de publicación: Germany
- Autores (p.o. de firma): B. de Celis, R. de la Fuente, A. Williart, B. de Celis Alonso

Título: *Coincidence measurements in  $\alpha/\beta/\gamma$  spectrometry with phoswich detectors using digital pulse shape discrimination analysis*

Ref. Nucl. Inst. Meth. Phys. Res. A

Volumen: A 580 pags. 206-209 Fecha: Mayo 2007

Lugar de publicación: Holland

- Autores (p.o. de firma): M. Shaw, A. Báguena, A. Williart, G. García

Título: *Development of an X-Ray installation for the study of secondary electrons: preliminary measurements and calculations*

Ref. Proceedings of “Second European IRPA Congress on radiation Protection”

Volumen: P-324 pag. 1-17 Fecha: Mayo 2006

Lugar de publicación: Paris

- Autores (p.o. de firma): A. Muñoz, A. Williart, G. García, J.M. Pérez

Título: *A new approach to the modeling of low energy gamma photon interaction in air*

Ref. Proceedings of “11<sup>th</sup> International Congress of the International Radiation Protection Association”

Volumen: 3b28 pag. 1-10 Fecha: Mayo 2004

Lugar de publicación: Madrid

- Autores (p.o. de firma): A. Roldán, J.M. Pérez, A. Williart, F. Blanco and G. García

Título: *Energy deposition model for low-energy electrons (0.01 - 10 keV) in air*

Ref. Journal of Applied Physics

Volumen: 95      Páginas, inicial: 5865    final: 5870      Fecha: Mayo 2004

Lugar de publicación: USA

## C.2. Congress,

- Título: *Low energy particle track simulation for biomedical applications*

Autores: M.C. Fuss, A.G. Sanz, A. Muñoz, J.C. Oller, F. Blanco, A. Williart, C. Huerga, M. Tellez and G. García

Tipo de participación: Oral

Congreso: “Radam 2010” (Radiation damage in biomolecular systems)

Lugar de celebración: Madrid      Fecha: 30 de junio – 4 de julio de 2010

- Título: *Analysis and modeling of secondary electron generation in condensed biomolecular systems*

Autores: A.G. Sanz, M.C. Fuss, A. Williart, C. Cruz, A. Perea, M.J.G. Borge, O.Tengblad, Y. Prezado, A. Muñoz, F. Blanco and G. García

Tipo de participación: Poster

Congreso: “Radam 2010” (Radiation damage in biomolecular systems)

Lugar de celebración: Madrid      Fecha: 30 de junio – 4 de julio de 2010

- Título: *LEPTS, una simulación de trayectorias de partículas de baja energía, en aplicaciones biomédicas*

Autores: M.C. Fuss, A.G. Sanz, A. Muñoz, J.C. Oller, F. Blanco, A. Williart, C. Huerga, M. Tellez y G. García

Tipo de participación: Oral

Congreso: XXXIII Reunión Bienal de la Real Sociedad Española de Física

Lugar de celebración: Santander      Fecha: 19-23 de septiembre de 2011

- Título: *Estudio de la absorción de las emisiones del Na<sup>22</sup> por distintos materiales.*

Autores: A. Williart, A. Muñoz, F. Blanco y G. García

Tipo de participación: Oral

Congreso: XXXIII Reunión Bienal de la Real Sociedad Española de Física

Lugar de celebración: Santander      Fecha: 19-23 de septiembre de 2011

### C.3. Research projects,

- Título del proyecto: “**Radiological EFfect of RAdicals and MolEcular Radiosensitisers (REFRAMER)**”  
Entidad financiadora: MICINN (PID20198-104727RB-C21)  
Entidades participantes: CSIC - UNED – CIEMAT- Universidad Complutense de Madrid  
Duración, desde: 2019 hasta: 2022  
Investigador responsable: G. García Gómez-Tejedor (CSIC)  
Número de investigadores participantes: 10
- Título del proyecto: “**Interacción de partículas de baja energía y radicales en aplicaciones biomédicas de la radiación**”  
Entidad financiadora: MINECO (FIS2016-80440-p)  
Entidades participantes: CSIC - UNED – CIEMAT- Universidad Complutense de Madrid  
Duración, desde: 2017 hasta: 2019  
Investigador responsable: G. García Gómez-Tejedor (CSIC)  
Número de investigadores participantes: 10
- Título del proyecto: “**Interacción de la radiación a escala nanométrica y sus aplicaciones en radioterapia y radiodiagnóstico**”  
Entidad financiadora: MINECO (FIS2012-31230)  
Entidades participantes: CSIC - UNED – CIEMAT- Universidad Complutense de Madrid  
Duración, desde: 2012 hasta: 2016  
Investigador responsable: G. García Gómez-Tejedor (CSIC)  
Número de investigadores participantes: 10
- Título del proyecto: “**Estudio de procesos atómicos y moleculares con aplicaciones en el uso biomédico de las radiaciones**”  
Entidad financiadora: CICYT (FIS2009-10245)  
Entidades participantes: CSIC - UNED – CIEMAT- Universidad Complutense de Madrid  
Duración, desde: 2009 hasta: 2012  
Investigadora responsable: G. García Gómez-Tejedor (CSIC)  
Número de investigadores participantes: 7
- Título del proyecto: “**Estudio del daño por radiación producido por electrones secundarios en sistemas biomoleculares**”  
Entidad financiadora: CSN  
Entidades participantes: UNED  
Duración, desde: 2004 hasta: 2009  
Investigadora responsable: M. Shaw Martos (UNED)  
Número de investigadores participantes: 2
- Título del proyecto: “**Interacción de electrones secundarios con la materia y sus implicaciones en el daño por radiación**”  
Entidad financiadora: CICYT (BMF04648/FISI)  
Entidades participantes: CSIC - UNED – CIEMAT- Universidad Complutense de Madrid  
Duración, desde: 2004 hasta: 2007  
Investigador responsable: G. García Gómez-Tejedor (CSIC)  
Número de investigadores participantes: 7

<b>Parte A. DATOS PERSONALES</b>		<b>Fecha del CVA</b>	10/10/2023
Nombre	Beatriz		
Apellidos	Galiana Blanco		
Sexo (*)		Fecha de nacimiento (dd/mm/yyyy)	
DNI, NIE, pasaporte			
Dirección email	Bgaliana@fis.uc3m.es	URL Web	
Open Researcher and Contributor ID (ORCID) (*)	0000-0001-9382-1278		

\* datos obligatorios

#### A.1. Situación profesional actual

Puesto	Profesora titular de Universidad		
Fecha inicio	23/02/2019		
Organismo/ Institución	Universidad Carlos III de Madrid		
Departamento/ Centro	Física		
País	España	Teléfono	916246261
Palabras clave	Células solares, caracterización de materiales fotovoltaicos, materiales luminiscentes, microscopía electrónica de transmisión		

#### A.2. Situación profesional anterior (incluye interrupciones en la carrera investigadora, de acuerdo con el Art. 45.2.c) de la convocatoria, indicar meses totales)

Periodo	Puesto/ Institución/ País / Motivo interrupción
2002-2006	Investigadora predoctoral (FPU), Instituto de Energía Solar-UPM, España
01-2007/06-2008	Investigadora posdoctoral, Instituto de Energía Solar-UPM, España
06-2008/01-2009	Investigadora invitada. Helmholtz Center for Materials and Energy, Berlín, Alemania (6 meses)
01-2009/06-2011	Investigadora Juan de la Cierva, Instituto de ciencia de Materiales de Madrid, ICMM-CSIC, España
07-2011/09-2012	Investigadora Posdoctoral, Ohio State University (EEUU) (14 meses)
09-2012/08-2017	Profesora Ayudante doctor. Dep. Física, Universidad Carlos III de Madrid, España
09-2017/-02-2019	Profesora Visitante. Dep. Física, Universidad Carlos III de Madrid, España
02-2019/	Profesora Titular. Dep. Física, Universidad Carlos III de Madrid, España

#### A.3. Formación Académica

Grado/Master/Tesis	Universidad/Pais	Año
Ingeniería Electrónica	Universidad Complutense de Madrid/España	2001
Doctorado	Universidad Politécnica de Madrid/España	2006

## Parte B. RESUMEN DEL CV (*máx. 5000 caracteres, incluyendo espacios*):

Beatriz Galiana es profesora titular del departamento de Física de la UC3M desde 2019. Actualmente es la directora del laboratorio de microscopía electrónica de transmisión (LABMET) perteneciente a la Red de la Comunidad de Madrid y la coordinadora del grupo de investigación reconocido por la UC3M “Materiales avanzados para aplicaciones en energía solar” en la UC3M que engloba a ocho investigadores. Dispone de una amplia experiencia investigadora en el campo de la energía solar y los dispositivos electrónicos, en el crecimiento epitaxial y caracterización avanzada de materiales. Es coautora del récord del mundo de células multiunión de dos uniones (GaInP/GaAs) y ha participado en el proyecto nacional coordinado (UPM, Universidad de Málaga, UC3M) TEC2014-54260- C3-3-P obteniendo células de tres uniones con 43% de eficiencia. Su tesis fue premiada a nivel europeo por la Catédrula Solfocus (2009). Ha realizado estancias de investigación en la Universidad Phillips de Marburg (Alemania), en el Hain Mainer Institute de Berlin (Alemania), en Ohio State University en Columbus (EEUU) y en el CINVESTAV del Instituto Politécnico Nacional de Ciudad de México juntando tres años de experiencia internacional. Ha publicado 52 artículos en revista JCR, 33 en primer cuartil, 44 publicaciones en congreso, con 851 citas totales y un factor h=16. Su carrera científica se ha desarrollado mediante contratos competitivos (FPU, Juan de la Cierva y José Castillejo (dos convocatorias) y en diferentes centros tanto nacionales (Instituto de Energía Solar-UPM, Instituto de Ciencia de Materiales del CSIC e IMDEA Materiales) como internacionales. Ha participado en 15 Proyectos nacionales y 5 internacionales. Actualmente es IP del proyecto Nacional “Análisis y desarrollo de materiales para su integración en células solares basadas en nanohilos III-V (DAMAINSOL)” con una financiación de (78.000 euros), y del “Desarrollo del Programa de actividades de I+d multidisciplinares del Centro de Tecnologías para la Fusión (TechnoFusión)” gestionando una cuantía de 140.000 euros. También es IP del proyecto financiado por la AECID en colaboración con la ONG Sopepaz, para la creación de un centro de formación profesional en Energías Renovables en Grand’Anse, Haití con una financiación de 530.000 euros. En el ámbito de las aportaciones a la sociedad, tiene dos patentes, una para el uso de cristales fotónicos en células solares y otra para la nanoestructuración de óxidos de alta permitividad (high-k) para electrónica de alta velocidad. Ha participado en cuatro contratos con la industria (Isofotón (2), La Mancha Solar e Intel Irlanda) y uno activo con SILBAT S.L.

En el ámbito de la formación es directora de la tesis doctoral de Amalia Navarro de Mesa, “Materiales semiconductores para aplicaciones en células solares fotovoltaicas. Caracterización mediante microscopía electrónica de transmisión (TEM).” (Lectura mayo 2022- Cum laude). Ha dirigido ocho trabajos fin de grado en el ámbito de la energía solar. Imparte docencia en el grado en Ingeniería de la Energía y en el máster universitario Ciencia e Ingeniería de Materiales de la UC3M juntando más de 1000 horas de docencia, de las cuales más del 90% han sido impartidas en inglés.

### C.1. Publicaciones más importantes en libros y revistas con “peer review” y conferencias

1. P.Tejedor, E. García-Tabarés, **B.Galiana**, L. Vazquez, B. J. García “Linear arrays of InGaAs quantum dots on nanostructured GaAs-on-Si substrates ” Applied surface Science, (156518), 2023 DOI: <https://doi.org/10.1016/j.apsusc.2023.156518>
2. E. Salas-Colera, M. Tardío, E. García-Tabarés, B. Perea, M. L. Crespillo, J.E. Muñoz-Santiuste, **B. Galiana**.“Development of Luminescent Nd-Doped LaNbO Compound Thin Film Growth by Magnetron Sputtering for the Improvement of Solar Cells” Crystals 2023, 13, 159. <https://doi.org/10.3390/cryst13020159>
3. A. Navarro. E. García-Tabarés, Q.M. Ramasses, **B.Galiana**, “Advanced transmission electron microscopy investigation of defect formation in MOVPE-growth of GaP on silicon using arsenic initial coverage” Applied surface Science, 610 (155578), 2023 DOI: <https://doi.org/10.1016/j.apsusc.2022.155578>
4. P.Cano; C. Ruiz, A. Navarro, **B. Galiana**, I.Garcia, I. Rey-Stolle “Growth of GaP Layers on Si Substrates in a Standard MOVPE Reactor for Multijunction Solar Cells” COATINGS (11)(2021) DOI:10.3390/coatings11040398

5. A.Mariscal-Jimenez, AT, Martin-Luengo, **B. Galiana**, C. Ballesteros, A. Bonanni, J. Martin-Sanchez, R. Serna "Photoluminescence and Stoichiometry Correlation in Nanocrystalline EuOx Thin Films: Tunable Color Emission", Journal of physical chemistry C, 124, pp: 15434-15439, (2020) DOI: 10.1021/acs.jpcc.0c03052
6. M.Fernandez-Alvarez, F.Velasco, A.Bautista, **B.Galiana** "Functionalizing organic powder coatings with nanoparticles through ball milling for wear applications" Applied Surface Science, 513, 145834, (2020). DOI: 10.1016/j.apsusc.2020.145834
7. M. Steidl, C.Koppka, **B. Galiana**. L. Winterfeld, K. Peh, B. O. Supplie, P. Kleinschmidt, E. Runge, T. Hannappel "Impact of Rotational Twin Boundaries and Lattice Mismatch on III-V Nanowire Growth" ACS Nano 11, (2017), <https://doi.org/10.1021/acsnano.7b01228>
8. V. Orlando,M. Gabas, **B. Galiana**, et al."Failure analysis on lattice matched GaInP/Ga(In)As/Ge commercial concentrator solar cells after temperature accelerated life test's. Progress in photovoltaics, 25 (1):97-112 (2017).
9. A Redondo-Cubero , B Galiana , K Lorenz , FJ Palomares , D Bahena , C Ballesteros, I Hernandez-Calderón and L Vázquez, "Self-organised silicide nanodot patterning by medium-energy ion beam sputtering of Si(100): local correlation between the morphology and metal content", Nanotechnology 27 (2016) 444001 (11pp). <https://doi.org/10.1088/0957-4484/27/44/444001>
10. T. J. Grassman, J. A. Carlin, **B. Galiana**, L.-M. Yang, F. Yang, M. J. Mills, S. A.Ringel, "Nucleation-Related Defect-Free GaP/Si(100) Heteroepitaxy via Metal-Organic Chemical Vapor Deposition", Applied physics letters, 112 (2013) 142102. <https://doi.org/10.1063/1.4801498>

## CONGRESOS

1. TITULO: *Developement of phosphor by magnetron sputtering for solar cells improvement* **B. Galiana**, E. Salas, J.E. Muñoz Santiuste, R.de la Cruz, M. M.Tardío, C. Kanyinda-Malu, S.Athanasiopoulos, E. García-Tabarés, G.Belén Perea, 49th IEEE Photovoltaic Specialist Conference (PVSC). Philadelphia 2022 TIPO DE PRESENTACIÓN: Oral
2. TITULO: "Advanced Characterization by spectral cathodoluminescence of 1eV GaInAs inverted" metamorphic solar cells", A.Navarro,.J. Jimenez, **B.Galiana**, CONGRESO: IEEE 43th 39th IEEE Photovoltaic Specialist Conference (PVSC). Virtual Meeting, su lugar inicial Calgary, Canada. (2020) TIPO DE PRESENTACIÓN: Póster
3. TÍTULO: "MOVPE growth of GaP on Si with As initial coverage", A.Navarro, E. García-Tabarés, **B. Galiana**, P. Caño, I. Rey-Stolle, C. Ballesteros, CONGRESO: 41th IEEE PVSC, San Diego, EEUU (2016). Poster
4. TÍTULO: "Nonuniversality due to inhomogeneous stress in semiconductor surface nanopatterning by low-energy ion-beam irradiation" A. Moreno; M. Castro; R. Gago; L. Vázquez; J. Muñoz-García; A. Redondo; **B. Galiana**; C. Ballesteros; R. Cuerno. CONGRESO: 8th International Workshop on Nanoscale Pattern Formation at surfaces, Cracovia, Polonia (2015). TIPO DE PRESENTACIÓN: Participativo - Ponencia invitada/ Keynote
5. TÍTULO: "Ideal GaP/Si Heterostructures Grown by MOCVD: III-V/Active-Si Subcells, Multijunctions, and MBE-to-MOCVD III-V/Si Interface Science" S. A. Ringel, J.A Carlin, T. J Grassman, **B. Galiana**, A. M Carlin, C.r Ratcliff et al. CONGRESO: 39th IEEE PVSC, Florida, EEUU (2013). TIPO DE PRESENTACIÓN: Poster

## C.3. Proyectos o líneas de investigación en los que ha participado.,

**Título del proyecto:** "Desarrollo del Programa de actividades de I+d multidisciplinares del Centro de Tecnologías para la Fusión (TechnoFusión)"  
Convocatoria de Programas de I+D Tecnologías 2018 (CM)  
Duración, 2019-2023. Cuantía de la subvención:140.000 €  
Investigador responsable: Beatriz Galiana (LAB 64)

**Título del proyecto** "Centro de formación profesional en Energías Renovables en el Grand'Anse, Haití.

Entidad financiadora: AECID+Universidad Unoga

Duración: 1/01/ 2020- 30/06/2022. Cuantía: 530.000 euros.

Investigador responsable: Beatriz Galiana

**Título del proyecto:** Análisis y desarrollo de materiales para su integración en células solares basadas en nanohilos III-V (DAMAINSOL)

Entidad financiadora: Ministerio de economía y competitividad

Duración, 2019 – 2022. Cuantía de la subvención: 78.000 €

Investigador responsable: Beatriz Galiana

**Título del proyecto:** Evaluación de arquitecturas de nueva generación en células solares multiunión para lograr eficiencias del 50%.

Entidad financiadora: Ministerio de economía y competitividad

Duración: 2014- 2017. Cuantía de la subvención: 70.000 €

Investigador responsable: Carmen Ballesteros.

Participación: Equipo de investigación (Caracterización TEM, AFM, SEM)

**Título del proyecto:** Epitaxia avanzada de semiconductores III-V para dispositivos nMOS altamente escalados (MAT2011-22536)

Entidad financiadora: MICINN-Proyectos de Investigación Plan Nacional I+D

Duración: 2012-2014 Cuantía: 70 K€

IP: Paloma Tejedor

Participación: Equipo de investigación (Crecimiento MBE, Caracterización TEM, AFM)

#### C.4. Participación en actividades de transferencia de tecnología/conocimiento y explotación de resultados

##### C.4. Contratos

Título del contrato: Caracterización avanzada de capas antirreflejantes para el infrarrojo

Empresa/administración financiadora: SILBAT

Duración desde Oct 2022 HASTA: Oct 2025

Investigador/a responsable: Beatriz Galiana

Título del contrato: Passivation of III-V semiconductor/high-k dielectric interfaces by hydrogen-assisted molecular beam epitaxy (H-MBE)

Empresa/administración financiadora:: Intel Corporation

Duración desde 2008 HASTA: 2011

Investigador/a responsable: Paloma Tejedor Jorge

Título del contrato: Adaptación de células solares multiunión a los concentradores F-DTIR

Empresa/administración financiadora: Concentración Solar la Mancha

Duración desde: Enero-2008 HASTA: Julio 2008

Investigador/a responsable: Carlos Algora

Título del contrato: Fabricación de estructuras de doble unión GaInP/GaAs por MOVPE

Empresa/administración financiadora: Isofotón S.A

Duración desde: Sept. 2004 HASTA: Noviembre 2005

Investigador/a responsable: Carlos Algora

##### C.5. Patentes

INVENTORES: C. Algora del Valle, I Andreani, F. Briones Fernandez-pola, B Galiana Blanco, M. Galli, , A. Rodriguez Alija "Solar cell for electric current generation device, has several ordered network of cavities that are formed on main surface and filled with air" (WO2009133225-A1; ES2346614-A1 ; ES2346614-B1)

FECHA 29-Abril-2008 ENTIDAD TITULAR: C.S.I.C., UPM y Universidad de Pavia

INVENTORES (p.o. de firma): P. Tejedor, M. Benedicto, B. Galiana

TITULO: Method for nano-structuring ultra thin sheets in e.g. industrial catalysts, involves transferring photo resist material to base substrate sheet, and placing organic waste in anti-reflection coating layer during reactive ion etching process (ES2395033-A1 ; ES2395033-B1)

FECHA DE PRIORIDAD: Mayo 2011 ENTIDAD TITULAR: C.S.I.C.

**Parte A. DATOS PERSONALES**
**Fecha del CVA** | 31/10/2023

Nombre y apellidos	Rafael José López Fernández	Edad	
DNI/NIE/pasaporte			
Núm. identificación del investigador	Researcher ID H-9216-2015 Código Orcid 0000-0002-9676-7534		

**A.1. Situación profesional actual**

Organismo	Universidad Autónoma de Madrid		
Dpto./Centro	Facultad de Ciencias		
Dirección	Avda Tomás y Valiente 7, módulo 14, desp. 611		
Teléfono		correo electrónico	
Categoría profesional	Profesor Titular	Fecha inicio	20-5-1988
Espec. cód. UNESCO	2206, 2207, 2208		
Palabras clave	Integrales moleculares, funciones de Slater, densidad electrónica		

**A.2. Formación académica (título, institución, fecha)**

Licenciatura/Grado/Doctorado	Universidad	Año
Lic. C. Químicas	Universidad Autónoma de Madrid	1980
Doctor Ciencias (Química)	Universidad Autónoma de Madrid	1986

**A.3. Indicadores generales de calidad de la producción científica (véanse instrucciones)**

Nº de sexenios: 6 (último concedido: período 2014-2019)

El ResearcherID recoge los siguientes registros que (aunque incompletos puesto que faltan las referencias a capítulos de libro y algunos artículos) da una idea razonable de mi métrica de citas:

Número de publicaciones recogidas: 89

Artículos con citas: 84

Número total de citas: 1644 (1155 sin autocitas)

Promedio de citas por artículo: 19.6

Factor h: 25

Citas anuales promedio últimos 5 años (excluido año actual): 55

Publicaciones en primer cuartil: 34 (15 J. Comput. Chem, 12 J. Chem. Phys, 7 Comput. Phys. Commun., 1 J. Chem. Theory Comput., 1 Royal Soc. Chem. Adv.)

**Parte B. RESUMEN LIBRE DEL CURRÍCULUM** (máximo 3500 caracteres, incluyendo espacios en blanco)

Mis investigaciones se han centrado en (1) el cálculo eficiente de integrales con funciones de Slater (STO) y su aplicación a los cálculos moleculares de alta calidad, (2) el análisis y la representación de la densidad electrónica molecular, (3) el estudio teórico de la estructura de los líquidos iónicos, y (4) el desarrollo de bases para cálculos moleculares.

Mi labor investigadora comenzó con el cálculo para integrales moleculares con funciones de calidad (funciones de Slater). Participé en el desarrollo y la programación de diversos algoritmos, que se plasmaron en un programa de cálculo completo para cálculos moleculares RHF con STO (SMILES), que sigue siendo una referencia en este tipo de investigaciones, como acredita la pervivencia en las citas (J. Comput. Chem., 19, 1284-1293, 1998). Esta línea de trabajo dio lugar a un contrato con la European Office of Aerospace Research & Development (EOARD), para la mejora de algoritmos de cálculo de integrales con funciones exponenciales.

Posteriormente comencé una línea de investigación sobre el reparto de la densidad electrónica molecular en contribuciones atómicas a partir de fragmentos atómicos definidos por la convergencia del potencial electrostático (MESP) de largo alcance. Este criterio conduce a fragmentos atómicos casi esféricos, con pequeñas deformaciones causadas por el entorno, y permite representar estos fragmentos de una manera que facilita enormemente el cálculo de propiedades relacionadas con la densidad electrónica, como son el MESP, el campo eléctrico y las fuerzas sobre los núcleos, facilitando la relación de los resultados

alcanzados mediante métodos de cálculo mecanocuánticos con los conceptos e interpretaciones de los estudios estructurales empíricos. Los algoritmos y programas desarrollados fueron recogidos en el paquete DAMQT, con posteriores versiones, en colaboración con el grupo del Prof. Gadre (Indian Institute of Technology at Kanpur, India), que incluyeron el análisis topológico de la densidad electrónica y del potencial electrostático molecular. Recientemente publicamos una nueva versión con algoritmos de cálculo más eficientes, y un interfaz gráfico más potente, con nuevos visores 2D y 3D y nuevas utilidades, como el análisis del MESP sobre superficies de densidad constante (*sigma holes*), y los desarrollos de la densidad en funciones de Canterakis-Zernike usados en identificación molecular, esto último en colaboración con los doctores G.B. Rocha y G. Urquiza-Carvalho de la Universidade Federal da Paraíba, Joao Pessoa, Brasil.

Con motivo de un proyecto de colaboración conjunta con sendos grupos de Ingeniería Química de la Universidad Complutense de Madrid (UCM) y la Universidad Autónoma de Madrid (UAM), me incorporé a la línea de investigación sobre líquidos iónicos iniciada por ambos grupos y liderada por los profesores Rodríguez Somolinos (UCM) y Palomar Herrero (UAM). Frutos de esta línea fueron las Tesis doctorales presentadas por la Dras. Del Olmo y Lage (esta última, premio de doctorado en la UAM). Finalmente, como colaborador del Dr. I. Ema y del Prof. García de la Vega (UAM) me he incorporado a la línea de investigación liderada por ambos sobre el desarrollo de nuevas bases para el cálculo de la estructura molecular.

Esta labor investigadora se ha complementado con las tareas docentes propias de mi situación laboral, e incluyen en estos últimos años la codirección de las dos tesis doctorales mencionadas, leídas en enero y en noviembre de 2016.

## Parte C. MÉRITOS MÁS RELEVANTES (ordenados por tipología)

### C.1. Publicaciones (últimos 10 años)

- (1) I. Ema, G. Ramírez, **R. López**, J.M. García de la Vega, ChemPhysChem, e202300485, doi.org/10.1002/cphc.202300485 (2023).
- (2) I. Ema, G. Ramírez, **R. López**, J.M. García de la Vega, J. Chem. Phys., 158, 244112 (2023).
- (3) S. Pathak, I. Ema, A.J. Lee, W.P. Bricker, **R. López**, S. Lehtola, J.A. Rackers, J. Chem. Phys., 158, 014104 (2023);
- (4) A. Kumar, **R. López**, F. Martínez, G. Ramírez, I. Ema, D. Zorrilla, Sachin D. Yeole, Shridhar R. Gadre, Comput. Phys. Commun., 279, 108460 (2022), “DAMQT 3: Advanced suite for the analysis of molecular density and related properties in large systems”.
- (5) I. Ema, G. Ramírez, **R. López**, J.M. García de la Vega, Computation, 10, 65 (2022), “Generation of Basis Sets for Accurate Molecular Calculations: Application to Helium Atom and Dimer”.
- (6) **R. López**, F. Martínez, J.M. García de la Vega, Theoretical Chemistry Accounts, 140, 18 (2021), “Molecular fingerprints based on Jacobi expansions of electron densities”.
- (7) B. Miguel, **R. López**, J.M. García de la Vega, Journal of Physics B: Atomic, Molecular and Optical Physics, 54, 025003 (2021), “Accurate atomic momentum integrals and Compton profiles”.
- (8) **R. López**, F. Martínez, I. Ema, J.M. García de la Vega, G. Ramírez, Computation, 7, 64 (2019), “Efficient Evaluation of Molecular Electrostatic Potential in Large Systems”.

- (9) G. A. Urquiza-Carvalho, G. B. Rocha, **R. López**, Journal of Computational Chemistry, 39, 2022-2032 (2018), “Efficient Algorithm for Expanding Theoretical Electron Densities in Canterakis-Zernike Functions”.
- (10) I. Lage, L. del Olmo, **R. López**, J.M. García de la Vega, Journal of Molecular Liquids, 256, 175–182 (2018), “Molecular modeling and physicochemical properties of 1-alkyl-3-methylimidazolium-FeX<sub>4</sub> and -Fe<sub>2</sub>X<sub>7</sub> (X = Cl and Br) magnetic ionic liquids”.
- (11) I. Lage, L. del Olmo, **R. López**, J.M. García de la Vega, Journal of Computational Chemistry, 38, 530–540 (2017), “The Role of Errors Related to DFT Methods in Calculations Involving Ion Pairs of Ionic Liquids”.
- (12) **R. López**, J. Fernández Rico, G. Ramírez, I. Ema, D. Zorrilla, A. Kumar, S. D. Yeole, S. R. Gadre, Comput. Phys. Commun., 214, 207:215 (2017), “Topology of molecular electron density and electrostatic potential with DAMQT”.
- (13) L. del Olmo, I. Lage, **R. López**, J.M. García de la Vega, The Journal of Physical Chemistry B, 120, 10327 (2016), “Understanding the Structure and Properties of Cholinium Amino Acid Based Ionic Liquids”.
- (14) A. Kumar, S. D. Yeole, S. R. Gadre, **R. López**, J. Fernández Rico, G. Ramírez, I. Ema, D. Zorrilla, J. Comput. Chem., 36, 2350:2359 (2015), “DAMQT 2.1.0: A New Version of the DAMQT Package Enabled with the Topographical Analysis of Electron Density and Electrostatic Potential in Molecules”.
- (15) L. del Olmo, I. Lage, **R. López**, J.M. García de la Vega, Royal Soc. Chem. Adv., 5, 72709 (2015), “Effect of dielectric constant on estimation of properties of ionic liquids: an analysis of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)- imide”.
- (16) **R. López**, J. Fernández Rico, G. Ramírez, I. Ema, D. Zorrilla, Comput. Phys. Commun., 192, 289-294 (2015), “DAMQT 2.0: A new version of the DAMQT package for the analysis of electron density in molecules”.
- (17) **R. López**, G. Ramírez, J.J. Fernández, I. Ema, J. Fernández Rico, Theor. Chem. Acc., 132: 1406:(1-10) (2013), “Multipole moments from the partition-expansion method”.
- (18) E.W. Hernández-Rodríguez, A.L. Montero-Alejo, **R. López**, E. Sánchez-García, L.A. Montero-Cabrera, J.M. García de la Vega, J. Comput. Chem., 34, 2460:2471 (2013), “Electron Density Deformations provide new Insights into the Spectral Shift of Rhodopsins”.
- (19) **R. López**, G. Ramírez, I. Ema, J. Fernández Rico, J. Comput. Chem., 34, 1800:1809 (2013), “Improved partition-expansion of two-center distributions involving Slater functions”.

## C.2. Proyectos

1. Referencia S2013/MAE-2800. "Título: Empleo de líquidos iónicos como alternativa a los disolvente orgánicos en procesos y productos", "Investigador principal: Francisco Rodríguez Somolinos (coordinador) y Rafael López Fernández (IP del grupo UAM2)", CAM, 10/2014-09/2018. 611.800€
2. Referencia S2009/PPQ-1545. "Título: Empleo de líquidos iónicos como alternativa a los disolvente orgánicos en procesos avanzados de separación", "Investigador principal: Francisco Rodríguez Somolinos (coordinador) y Rafael López Fernández (IP del grupo UAM2)", CAM, 01/2010-12/2013. 556.950€.

3. Referencia CTQ2010-19232. "Título: Estructura electrónica molecular: Metodología y Aplicaciones", "Investigador principal: José Manuel García de la Vega, MICINN, 01/2011-12/2013. 66.550€.
4. Referencia A1/035856/11. "Título: Centro virtual de Bioinformática: Formación de especialistas y creación científica", "Investigador principal: José Manuel García de la Vega", MAEC-AECID, 01/2012-12/2012. 72.500€.
5. Referencia D/030752/10. "Título: Centro virtual de Bioinformática: Formación de especialistas y creación científica", "Investigador principal: José Manuel García de la Vega", MAEC-AECID, 01/2011-12/2011. 65.900€.
6. Referencia D/0236653. "Título: Centro virtual de Bioinformática: Formación de especialistas y creación científica", "Investigador principal: José Manuel García de la Vega", MAEC-AECID, 01/2010-12/2010. 53.500€.
7. Referencia CTQ2007-63332. Título: Estructura electrónica molecular", "Investigador principal: José Manuel García de la Vega", MEC, 01/10/2007-30/09/2010. 95.590€

### C.3. Contratos, méritos tecnológicos o de transferencia

1. Referencia Grant 093069. "Título: Molecular Slater Integrals for Electronic Energy Calculations", "Investigador principal: Rafael López Fernández", EOARD, 09/2009-08/2010. 29.900 USD.

### C.4. Patentes

### C.5, C.6, C.7...

Miembro del Comité Internacional de Organización del MESBA 2016



## Part A. PERSONAL INFORMATION

CV date

27/10/2023

First and Family name | Pedro Córdoba Torres

Researcher numbers | Researcher ID | L-5280-2014

| Orcid code | 0000-0003-2006-1938

## A.1. Current position

Name of University/Institution	Universidad Nacional de Educación a Distancia		
Department	Dpto. de Física Matemática y de Fluidos/Facultad de Ciencias		
Phone number	913987141	E-mail	<a href="mailto:pcordoba@dfmf.uned.es">pcordoba@dfmf.uned.es</a>
Current position	Profesor Titular	From	27/07/2020
Espec. cód. UNESCO	2210		
Palabras clave	Physical chemistry of interfaces. Far-from equilibrium growth. Kinetic roughening. Random media. Random metrics. Electrochemical processes. Electrochemical impedance spectroscopy.		

## A.2. Education

Title	University	Year
MSc in Physics (Theoretical Physics)	Universidad Autónoma de Madrid	1996
PhD. Thesis in Physics (European Doctorate Mention)	Universidad Nacional de Educación a Distancia	2005

## A.3. JCR articles, h Index, thesis supervised...

- 4 CNEAI six-year research periods (sexenios): (1998-2004), (2005-2010), (2011-2016), (2017-2022).
- 23 JCR articles:
  - Publications in: D1=3, Q1=18, T1=23.
  - Single author in 5 publications, first author in 22.
  - Average number of citations per article: 39.5 (source: Scholar)
  - H-index: 16 (source: Scholar).

## Part B. CV SUMMARY

- (1998-2001) FPU predoctoral fellowship funded by the *Ministerio de Educación y Cultura*.
- Academic positions (all at *Departamento de Física Matemática y de Fluidos*, UNED):
  - (2001-2003): Adjunct Professor (*Prof. Asociado LRU a tiempo parcial*)
  - (2003-2006): Assistant Professor (*Prof. Ayudante LOU*)
  - (2006-2009): Tenure Assistant Professor (*Prof. Colaborador*)
  - (2009-2020): Associate Professor (*Prof. Contratado Doctor*)
  - (2020-present): Associate Professor (*Prof. Titular*)
- 6 Pre-doctoral research stays abroad (with a total duration of 11 months) funded by the short-term stays abroad program of the *Ministerio de Educación y Cultura*:
  - 2 stays (2.5 months) at the *Service de Physique Statistique, Plasmas et Optique Non-Linéaire, Université Libre de Bruxelles* (Belgium).
  - 1 stay (3 months) at the *Max Planck Institut für Molekulare Physiologie*, Dortmund (Germany).
  - 2 stays (5 months) at the *Centro de Tecnología de la COPPE, Universidade Federal do Rio de Janeiro* (Brazil).
  - 1 stay (0.5 months) at the *Instituto de Investigaciones Físico-químicas Teóricas y Aplicadas*, La Plata (Argentina).



- 2 Post-doctoral research stays abroad with a total duration of 8 months at the *Laboratoire d'Electrochimie et de Physico-chimie des Matériaux et des Interfaces* (Grenoble Institut of Technology-INPG, France). The longest one (6.5 months) was funded by the program "José Castillejo" for mobility and stays abroad for young postdoctoral researchers of the *Ministerio de Educación y Ciencia*.
- Participation as a researcher in the European Research & Innovation Contract *Computer Algebra Tools for Handling Ordinary Differential Equations*, Contract Networks of Excellence/ESPRIT 2. Working Group 24490. Funded by Commission of the European Communities Directorate-General for Industry (DGIII). Duration: from 01/05/1997 to 01/05/2000.
- Participation as a researcher in 8 projects with public funding (national: 5, autonomic: 1, UNED's research program: 2).
- 15 Contributions to international meetings:
  - 8 posters.
  - 4 oral communications.
  - 1 invited oral communication:
    - *New Insights on the Constant-Phase Element Behavior in Electrochemical Impedance Spectroscopy*, 65th Annual Meeting of the International Society of Electrochemistry (Lausanne, Switzerland), 31/08/2014 - 05/09/2014.
  - 2 invited plenary lectures:
    - *Computational modeling in surface growth processes: Dynamics of surface roughness*, X Encontro de Modelagem Computacional (Nova Friburgo, Brazil), 21-13/11/2007.
    - *Simulation de l'impédance par Monte-Carlo. Dissolution anodique en deux étapes consécutives. De l'interface lisse 2-D à l'interface rugueuse 3-D et ses effets de relaxation de surface*, 22ème Forum sur les impédances électrochimiques (Paris, France), 18/01/2010.
- Lines of research:
  - Far-from-equilibrium growth.
  - Stochastic geometry of growing surfaces (kinetic roughening).
  - Heterogeneous chemistry of electrochemical systems.
  - Electrochemical impedance spectroscopy of disordered systems: theory, modelling and experiments. Constant-phase element (CPE) behavior.
  - Growth in disordered media. Random metrics.
  - First-Passage Percolation: theory and applications.
  - Traffic flow dynamics.

## Part C. RELEVANT MERITS

### C.1. Publications (including books)

- Next publication is the first result of a collaboration I started a few years ago with the aim of studying the effect of the quenched disorder caused by random metrics on kinetic roughening. The results of this research led to the establishment of a line of research that was recognized with the award of a national project (PGC2018-094763-B-I00), which we hope will continue with another project that is currently in the evaluation process.

1. Pedro Córdoba-Torres, Silvia N. Santalla, Rodolfo Cuerno, Javier Rodríguez-Laguna, "Kardar–Parisi–Zhang universality in first-passage percolation: the role of geodesic degeneracy", *Journal of Statistical Mechanics: Theory and Experiment* (2018) 063212.



- In these works I presented a theory for the impedance response of different types of distributed systems: dielectric thin-films (2-4) and electrode surfaces (5), and provided a mathematical description for different anomalous behaviors found in the literature, paying special attention to ubiquitous and controversial CPE behavior:

2. P. Córdoba-Torres, "A general theory for the impedance response of dielectric films with a distribution of relaxation times", *Electrochimica Acta* **282** (2018) 892-904.
3. P. Córdoba-Torres, "A generalized expression for the resistivity distribution in films: from the Young model to constant-phase element (CPE) behavior", *Electrochimica Acta* **241** (2017) 535-543.
4. P. Córdoba-Torres, "Relationship between constant-phase element (CPE) parameters and physical properties of films with a distributed resistivity", *Electrochimica Acta* **225** (2017) 592-604.
5. P. Córdoba-Torres, "Characterization of frequency dispersion in the impedance response of a distributed model from the mathematical properties of the distribution function of relaxation times", *Electrochimica Acta* **180** (2015) 591-603.

- Next work has received a great attention by the physical-chemistry community (127 citations in Scholar) because it provides strong experimental evidences on the origin of the power-law CPE behavior found in the frequency response of electrodes and interfaces:

6. P. Córdoba-Torres, T.J. Mesquita, R.P. Nogueira, "Relationship between the origin of constant-phase element behavior in electrochemical impedance spectroscopy and electrode surface structure", *The Journal of Physical Chemistry C* **119** (2015) 4136–4147.

- Next is my most cited paper (159 citations in Scholar) as it proves the coupling of the two parameters involved in the mathematical definition of the CPE, a distributed model used extensively to interpret the EIS response of a wide variety of systems:

7. P. Córdoba-Torres, T.J. Mesquita, O. Devos, B. Tribollet, V. Roche, R.P. Nogueira, "On the intrinsic coupling between constant-phase element parameters alpha and Q in electrochemical impedance spectroscopy", *Electrochimica Acta* **72** (2012) 172-178.

- This is book chapter in which we present a review of the results obtained from the modeling and simulation of metal dissolution, with special attention to the coupling between the stochastic surface geometry and the surface distribution of chemical species:

8. P. Córdoba-Torres and R. P. Nogueira, *Modelagem computacional da dissolução metálica - Interfaces de eletrodos: Estrutura da superfície*, in I. Bastos, F. Moura Neto, N. Henderson, G. Platt and M. Rocha (Eds.), *Modelagem Computacional em Materiais, Ciência Moderna Ltda.*, Rio de Janeiro (2010) 235-256. ISBN: 978-85-7393-957-6.

- This work represents the main contribution of the author to the dynamic scaling theory in kinetic roughening, as it shows the first experimental evidence of the theoretically-conjectured faceted anomalous scaling:

9. P. Córdoba-Torres, T. J. Mesquita, I. N. Bastos, y R. P. Nogueira, "Complex Dynamics during Metal Dissolution: From Intrinsic to Faceted Anomalous Scaling", *Physical Review Letters* **102** (2009) 055504.

- Finally, I want to mention a relevant work in which, for the first time, the coupling between the relaxation of the surface morphology of a growing interface and the relaxation of the adsorbed species of a complex reaction mechanism was addressed:

10. P. Córdoba-Torres, M. Keddam y R. P. Nogueira, "On the intrinsic electrochemical nature of the inductance in EIS - A Monte Carlo simulation of the two-consecutive



steps mechanism: The rough 3 D case and the surface relaxation effect", *Electrochimica Acta* **54** (2009) 6779-6787.

## C.2. Research projects

IP and IP2 of the following projects (respectively):

-Title: *Efectos de escala sobre las medidas de impedancia electroquímica local y global en procesos de disolución metálica.*

-Funding entity: Vicerrectorado de Investigación de la UNED, Plan Propio de Promoción de la Investigación de la UNED (2010).

-Reference: 2010V/PUNED/0003.

-IP: Pedro Córdoba Torres.

-Affiliation entity: UNED.

-Duration: from 01/07/2010 to 30/06/2012.

-Funding: 3.000 euros.

-Title : *Simetría y geometría en las fluctuaciones de sistemas espacialmente extensos lejos del equilibrio.*

-Funding entity: Plan Nacional de Proyectos de I+D de GENERACIÓN DE CONOCIMIENTO (2018).

-Reference: PGC2018-094763-B-I00.

-IP1: Rodolfo Cuerno Rejado (UC3M).

-IP2: Pedro Córdoba Torres.

-Affiliation entity: Universidad Carlos III de Madrid.

-Duration: from 01-01-2019 to 31-12-2021.

-Funding: 40.000 euros.

## C.5. Review of works for scientific JCR journals

- Reviewer of *Electrochimica Acta*, *The Journal of Physical Chemistry and Condense Matter Physics*.

## C.6. Formative Activities

- Supervisor of the Degree's Thesis (TFG) in the Bachelor's Degree in Physics (Faculty of Sciences, UNED).

- Supervisor of the Master's Thesis (TFM) in: Master's Degree in Physics of Complex Systems, Master's Degree in Advanced Physics, and Master's Degree in Medical Physics (Faculty of Sciences, UNED).

- Supervisor of 2 contracts with public funding:

Contract: Predoctoral researcher.

Reference: PEJD-2018-PRE/IND-9095.

Funding entity: Comunidad de Madrid, co-funded by the European Social Fund (ESF) through the Youth Employment Operational Program (YEOP) and the Youth Employment Initiative (YEI) (2008).

Name of the researcher: Daniel Villarrubia Moreno.

Duration: from 01/03/2019 to 28/02/2021.

Contract: Research assistant.

Reference: PEJ-2018-AI/IND-10573.

Funding entity: Comunidad de Madrid, co-funded by the European Social Fund (ESF) through the Youth Employment Operational Program (YEOP) and the Youth Employment Initiative (YEI) (2008).

Name of the researcher: Iván Álvarez Domenech.

Duration: from 01/04/2019 to 31/03/2021.