



## Ramón Cuadrado del Burgo

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## Summary of CV

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

Dr. Cuadrado is an expert in the field of **first principles and multiscale simulations of the geometric, electronic and magnetic properties of nanomaterials**, ranging from molecular magnets, Carbon-based nano-materials, two-dimensional (2D) materials, disordered compounds to adsorption of molecules on surfaces. He uses and develops cutting-edge Density Functional Theory (DFT) techniques to achieve high accuracy in his predictions such as Spin-Orbit Coupling (SOC) and spin constrained-DFT (CDFT). His ability as an independent researcher is widely and internationally recognised. At Catalan Institut of Nanoscience and Nanotechnology (ICN2 – Barcelona) he currently hold a competitive **Marie Curie Intra-European COFUND personal grant ( P-Sphere)**. Previously, Dr. Cuadrado obtained an **Institutional Marie Curie European Fellowship** at The University of York (United Kingdom) and he was involved in several industry-facing projects with **Seagate, Samsung** and **Toyota**. At ICN2-UAB, he supervised the final project research of one last year undergraduate student, he delivered a practical session at the SIESTA School at Barcelona Supercomputer Center (BSC) regarding the new fully-relativistic implementation within SIESTA and he **organised and delivered a three days Open Knowledge Workshop about Magnetism methods in DFT** to PhD's and Master's students: "Spin-Orbit Coupling in SIESTA: Magnetism and other capabilities". During his first postdoctoral position at the University of York, he taught Lagrangian Mechanics, Newtonian Mechanics and Physics of Matter undergraduate courses and he co-supervised 2 PhD students. Dr. Cuadrado has published in international peer-reviewed journals of high impact factor (IF) such as Advanced Functional Materials (IF 13.325), Nature Communications (IF 12.353) and Physical Review Letters (IF 8.839), reaching **h-index = 9** and more than **200 citations** (SCOPUS). He has **11 first author papers** and **one invited paper** in Journal of Physics: Materials. It is worth mentioning that he is proactive in building and sustaining his own international network of excellent experimental and theoretical collaborators.

Since June 2015 he is working at the ICN2 in Barcelona in the "Theory and Simulation" group of Prof. Pablo Ordejón. His duties in the group were initially the implementation and optimisation, within the newest SIESTA version, the SOC adapted to the new MPI libraries and to update the official manual and tests. Aside of his current programming commitments, he is developing his personal Marie Curie project which is related with the study of bi-magnetic nano-systems. In this regard, he has successfully developed and implemented the noncollinear spin constrained-DFT with a fully relativistic Hamiltonian following its validation by means of different systems such as vanadium oxyfluoride V<sub>7O<sub>6</sub>F<sub>18</sub></sub>, Fe/graphene/Co/Ir(111) or calculating the magnetic exchange interactions of an infinite Fe chain by mapping the total self-consistent energy to a generalised Heisenberg spin model. The study of Fe/graphene/Co/Ir(111) interlayer coupling in collaboration with the experimental group of Dr. M. Valvidares of the ALBA Synchrotron Facility in Barcelona led to a recent Nature Communication publication. Furthermore, he has created and maintained a professional network composed of several



research groups such as Prof. Jordi Sort of the UAB, Prof. R. Chantrell of The University of York and Prof. L. Szunyogh of the University of Budapest, Hungary.

## General quality indicators of scientific research

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

**H index = 9, citations > 200** [Scopus, 25/1/2019]

Number of **publications = 24**

Publications as a **first author = 11**

**1** Invited paper at **Journal of Physics: Materials**: "Implementation of non-collinear spin constrained-DFT with a fully relativistic Hamiltonian"

### Invited talks and international conferences:

2 Invited talks in workshops: ALBA Synchrotron and at The University of Konstanz

1 Industry invited talk at **Toyota Motor Corporation** (Japan)

~20 conference presentations (9 oral and 11 poster)

**Chair** at InterMag Conference Dresden 2014: "ab-initio and transport II"

### Individual research grants:

- Personal Training Researcher Fellowship (FPI) Spanish Ministry of Science (2006-2010)

- Marie Curie Institutional Fellowship at The University of York, York, United Kingdom (2011-2013)

- Marie Curie Intra-European COFUND Fellowship at the ICN2-UAB (2016-2019)

### DFT-based implementation methods:

- Off-site Spin-Orbit Coupling in GREEN-SIESTA package.

- On-site Spin-Orbit Coupling in the official SIESTA package.

- Off-site Spin-Orbit Coupling in the official SIESTA package.

- Non-collinear spin constrained-DFT with a fully relativistic Hamiltonian.

### Outreach, teaching and dissemination activities:

Undergraduate:

- First year problem classes at The University of York: Newtonian Mechanics and Physics of Matter.

- Second year tutorials and problem classes: Lagrangian Mechanics

Postgraduate:

- Final degree project of Joaquim Iguaz at Autonomous University of Barcelona (UAB), Barcelona, Spain

- Invited to the **SIESTA School at Barcelona Supercomputer Center (BSC)** in May 2017 to introduce the new fully-relativistic implementation in the code.



- Organised and delivered three days **Open Knowledge Workshop** at ICN2 (May 2018) about magnetism capabilities of SIESTA.



## Ramón Cuadrado del Burgo

Surname(s): **Cuadrado del Burgo**  
 Name: **Ramón**  
 ORCID: **0000-0002-8344-2319**  
 ResearcherID: **H-9543-2015**

### Current professional situation

**Employing entity:** Institut Català de Nanociència i Nanotecnologia (ICN2-CSIC) **Type of entity:** Foundation  
**Department:** Institut Català de Nanociència i Nanotecnologia  
**Professional category:** Marie Curie Incoming **Educational Management (Yes/No):** Yes  
 COFUND Postdoctoral Research  
**City employing entity:** Barcelona, Catalonia, Spain  
**Phone:** (0034) 937373624 **Email:** ramón.cuadrado@icn2.cat  
**Start date:** 15/06/2015

**Type of contract:** Grant-assisted student (pre or post-doctoral, others) **Dedication regime:** Full time

**Primary (UNESCO code):** 220305 - Electron states; 220306 - Electron transport; 221102 - Composites; 221105 - Crystal structure; 221110 - Electron states; 221111 - Electron transport properties; 221112 - Imperfections; 221114 - Interfaces; 221115 - Lattice mechanics; 221117 - Magnetic properties; 221119 - Mechanical properties; 221123 - Non-crystalline states; 221126 - Solid state devices; 221190 - Solid state Physics. Foil

**Performed tasks:** Since 2015 I am working in the "Theory and Simulation" group of Prof. Pablo Ordejón at the Catalan Institute of Nanoscience and Nanotechnology (ICN2) in Barcelona. My duties in the group were initially the implementation and optimisation, within the newest SIESTA version, the off-site Spin-Orbit coupling (SOC) approximation adapted to the new MPI libraries and to update the official manual and tests. Aside of my current programming commitments, I am developing my personal Marie Curie project which is related with the study of bi-magnetic nanosystems. In this regard, I have successfully developed and implemented the noncollinear spin constrained-DFT (CDFT) with a fully relativistic Hamiltonian following its validation by means of different systems such as vanadium oxyfluoride V<sub>7O<sub>6</sub>F<sub>18</sub></sub>, Fe/graphene/Co/Ir(111) or calculating the magnetic exchange interactions of an infinite Fe chain by mapping the total self-consistent energy to a generalised Heisenberg spin model. The study of Fe/graphene/Co supported on Ir(111) substrate in collaboration with the experimental group of Dr. M. Valdivares (ALBA Synchrotron Facility in Barcelona) led to the publication of an article in Nature Communication journal and as a main result we unveiled the interlayer superexchange-coupling between Fe and Co magnetic monolayers mediated by graphene.

**Field of management activity:** University

**Applicability in teaching and/or research:** During the past ten years I have gained a wide range of teaching experience in physics and mathematics, at different undergraduate and postgraduate levels in Spain and in the UK. In May 2017 I was invited to be part of the SIESTA school instructors that was held at Barcelona Supercomputing Center (BSC) to introduce to PhD students and to experimental researches the new magnetic capabilities of the SIESTA code bringing me the opportunity to introduce them in the fascinating world of modeling experiments from first principles. The lectures were theoretical sessions during the morning and hands-on in the afternoon. This gave me the opportunity to show my recent implemented fully relativistic approximation and motivated me to prepare and execute the course material in an engaging manner to a different type of audience.

**Previous positions and activities**

	<b>Employing entity</b>	<b>Professional category</b>	<b>Start date</b>
<b>1</b>	The University of York	Postdoctoral Research Assistant	01/05/2011
<b>2</b>	Instituto de Ciencia de Materiales de Madrid	PhD Student	01/08/2006

- 1** **Employing entity:** The University of York      **Type of entity:** University  
**Department:** Physics, Physics  
**City employing entity:** The University of York, North Yorkshire, United Kingdom  
**Professional category:** Postdoctoral Research Assistant      **Educational Management (Yes/No):** Yes

**Start-End date:** 01/05/2011 - 15/06/2015      **Duration:** 4 years - 1 month - 15 days

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

**Dedication regime:** Full time

**Primary (UNESCO code):** 221102 - Composites; 221105 - Crystal structure; 221110 - Electron states; 221111 - Electron transport properties; 221114 - Interfaces; 221117 - Magnetic properties; 221119 - Mechanical properties; 221126 - Solid state devices; 221190 - Solid state Physics. Foil; 221199 - Other

**Performed tasks:** After finishing my doctorate at ICMM-CSIC in Madrid, I was funded by a Marie Curie Institutional fellowship allowing me to move to the UK and begin my first postdoctoral research position at The University of York under the supervision of Prof. Roy W. Chantrell. During my time in York I have been involved in number of projects both industrial and purely scientific such as "MagHEM" (Toyota Motor Corporation) and "Atomistic Simulation of Advanced Materials for MRAM applications" (Samsung) or Mahasarakham University in Thailand. As the sole member of the group with a background in electronic structure theory my involvement in each of these projects was to handle all aspects of the ab initio, molecular dynamics, and DFT and post-DFT techniques using DFT+U or DFT+vdW, to support the multiscale modelling. Importantly, for industrial applications is understanding of the electronic structure of complex interfaces and how they might behave. Such insight is usually not accessible by experimental methods, making the approaches that I use through DFT of paramount importance to our industrial collaborators. A Seagate technology, The University of York's principal research partner, is one of the most active hard-drive manufacturers in the world and developer of high-density magnetic recording technology. In this regard, I was responsible for carrying out first principles calculations involving the technologically relevant FeXPt-L1\_0 in molecular, interfacial and bulk phases. By means of the fully relativistic formalism implemented in SIESTA I am able to calculate, with a high accuracy, the magnetic anisotropy energy (MAE) of such systems. In one particular project, I performed a structural, electronic and magnetic survey of bimetallic cuboctahedral nanoparticles (NPs) from 13 up to 147 atoms. The aim of the study was to determine the size and compositional dependence of the thermal stability arising from the anisotropy. As well as NP systems, the behaviour of FePt (and other materials) when it is interfaced with different materials, such as MgO or bcc-Fe, is an area of current interest. MgO substrates possess the ability to keep its optimized in-plane lattice almost unchanged when it is brought into contact with Fe or FePt. This allows one to fix the 2D values and tune the out-of-plane c/a ratio of the other alloys proving ways of engineering desirable properties. Another possibility to tune the MAE of bulk phases is by doping several non-magnetic species such as Mn, Cu or Cr instead of Fe. This has been experimentally demonstrated and corroborated in a recent publication in Applied Physics Letters that I performed in collaboration with Seagate. Finally, as initial step to shed light on how materials grow on surfaces, I studied the wettability of the MgO (001) surface taking into account different sizes and adsorption sites for small FePt clusters. A whole knowledge of magnetic materials would not be complete without the possibility to obtain the magnetic exchange interactions. Such calculations are very challenging, particularly the ability to determine the whole exchange tensor. Through an on-going collaboration with Laszlo Szunyogh I have more recently been involved in using the Wein/Budapest-SKKR code.



**Field of management activity:** University

**Applicability in teaching and/or research:** During my first postdoctoral position at The University of York I was in charge of delivery tutorial and problem classes of Newtonian Mechanics, Physics of Matter and Lagrangian Mechanics, first and second year undergraduate studies, respectively. As speaker, I have pursued to provide the students with useful analytical skills in each subject, including the ability to think and express oneself logically and the capability to learn outside the traditional classroom setting. I attempted to do so focusing on applied examples and by providing appropriate opportunities for students to practice and develop independent learning skills through methods such as simple research projects or investigative team work. My aim has been always to foster a general understanding and appreciation for the world around us, not just in the academic environment, but also in their future professional career.

**2 Employing entity:** Instituto de Ciencia de Materiales de Madrid

**Type of entity:** State agency

**Professional category:** PhD Student

**Educational Management (Yes/No):** No

**Start-End date:** 01/08/2006 - 30/04/2011

**Duration:** 4 years - 8 months

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

**Performed tasks:** During my time at the ICMM-CSIC in Madrid I started to work as PhD within the joint project “Dinámica y Electrónica de Espín en Nanomateriales: Estructuras Epitaxiales Crecidas por MBE y Modelización” in the experimental group of Prof. Jesús M. Gonzalez. I started to build my magnetism expertise by means of fabricating different types of magnetic multilayered systems using the Pulse Laser Deposition (PLD) technique, characterizing their structure by a X-ray diffractometer and finally the magnetic properties by means of the Vibrating Sample Magnetometer (VSM) [24-26]. These initial works were based in the study of different ordered and disordered magnetic phases, magnetic properties and their thermal dependence as well as the hysteretic behaviour of LaMnO<sub>3</sub> and SmCo compounds. Next, I commenced to work with Dr. J. Iribas Cerdá and I focused my research to the theoretical description of magnetic materials by means of the use of DFT, post-DFT and Quantum Molecular Dynamics techniques. A significant portion of my work was related to the implementation and optimisation of the off-site Spin-Orbit Coupling (SOC) interaction into the GREEN-SIESTA DFT package under the Pseudopotential (PP) approximation. To this end, the formalism was developed to obtain the total Hamiltonian in its fully relativistic form by means of the radial solutions of the Dirac equation. Hence, the total Hamiltonian involves not only the Darwin and velocity-correction term but also the SOC term. Such improvement of the GREEN-SIESTA code covers such important physical aspect not previously available. This has enabled me to study fully relativistic effects on the electronic structure of a wide number of technologically relevant magnetic materials. In addition to the implementation of the SOC interaction, I also carried out research looking at the adsorption of organic C<sub>60</sub> and CoPc molecules onto Si(111) and Cu(111) surfaces, respectively. To this end, I performed a wide range of possible geometric adsorption sites with the aim to obtain geometric ground states and furthermore corroborate the STM images. Specifically, the CoPc organic molecule loses its C<sub>4</sub> symmetry to C<sub>2</sub> upon adsorption on Cu. We successfully reproduced these experimental results in our calculations. Other relevant research that I performed was the study of thiol-capped gold nanoparticles. Apart from the lack of atomic geometric information, specifically when it takes into account bigger sizes, their intriguing magnetic behaviour is not yet understood. Many of the experimental findings prove contradictory with only a limited number of published theoretical works. I carried out a deep survey on the structure taking into account three core shapes and different thiol coverings. The metastable geometries were calculated performing molecular dynamics optimizations using simulated annealing. Subsequently, the electronic and magnetic properties were analysed.

**Field of management activity:** University





## Education

### University education

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

**University degree:** Higher degree

**Name of qualification:** Licenciado en Ciencias Físicas

**Degree awarding entity:** Universidad Complutense de Madrid **Type of entity:** University

**Date of qualification:** 10/10/2003

#### Doctorates

**Doctorate programme:** Doctor por la Universidad Autónoma de Madrid dentro del Programa oficial de posgrado en física de la materia condensada y nanotecnología

**Degree awarding entity:** Universidad Autónoma de Madrid **Type of entity:** University

**Date of degree:** 21/01/2011

### Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
English	C2	C2	C2	C2	C2

## Teaching experience

### General teaching experience

- Name of the course:** Heat and Matter/1  
**University degree:** Bs in Physics  
**Start date:** 01/10/2014 **End date:** 20/12/2014  
**Entity:** The University of York **Type of entity:** University  
**Faculty, institute or centre:** The Department of Physics
- Name of the course:** Lagrangian Mechanics/2  
**University degree:** Bs in Physics  
**Start date:** 01/10/2014 **End date:** 20/12/2014  
**Entity:** The University of York **Type of entity:** University  
**Faculty, institute or centre:** The Department of Physics



## Experience supervising doctoral thesis and/or final year projects

**Project title:** Geometric, electronic and magnetic study of Fe<sub>3</sub>O<sub>4</sub> nanoparticles by means of density-functional-based calculations

**Entity:** Universitat Autònoma de Barcelona

**Type of entity:** University

**Student:** Joaquim Iguaz Juan

**Date of reading:** 09/07/2018

## Scientific and technological experience

### Scientific or technological activities

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

- Name of the project:** Multiscale modeling of the interface in bi-magnetic nanosystems

**Entity where project took place:** FUNDACION PRIVADA INSTITUT CATALA DE NANOTECNOLOGIA

**City of entity:** Barcelona, Catalonia, Spain

**Name principal investigator (PI, Co-PI....):** Ramón Cuadrado del Burgo; Pablo Ordejón Rontomé

**Nº of researchers:** 2

**Funding entity or bodies:**  
European Community (FP7)

**Start-End date:** 01/07/2016 - 30/06/2019

**Total amount:** 149,7 €

**Applicant's contribution:** I identified two challenging key aspects to be addressed within this project: 1) Development of a complete mathematical framework capable of calculating all possible magnetic properties at the local level of nanosystems of arbitrary geometry: I proposed combining ab initio calculations with atomistic spin models, where the atoms are treated as possessing a local magnetic moment, macroscopic properties such as the Curie temperature, temperature-dependent anisotropies, and magnetic ground states, would be accessible from first principles electronic structure calculations. The generalised Heisenberg atomistic spin model encapsulates the essential physics of a magnetic material at the atomic level and it is typically written as a sum of various energy contributions or different origins (exchange, anisotropy, demagnetizing field, etc). The dominant term is the magnetic exchange energy typically up to 1000 times larger than the next largest contribution and gives rise to magnetic ordering. So here I proposed to outline a novel method based on fully-relativistic non-collinear spin CDFT based calculations in which the magnetic exchange interactions may be calculated mapping the generalised Heisenberg model to a total selfconsistent energy obtained with SIESTA. 2) Understanding of the physical interfacial phenomena, when two or more distinct materials with different magnetic ordering form a nanostructured entity, by means of a multiscale modeling. Due to that the main theoretical models are supported in Monte Carlo methods neglecting for example, the interface roughness or the spin structure at atomic level, I planned the development a more realistic theoretical model that permits the understanding of the MP novel effects in any bi-magnetic nanosystem with high relevant technological applications as well as from a fundamental point of view.
- Name of the project:** Simulaciones atomísticas de primeros principios: Metodología y aplicaciones en nanociencia

**Entity where project took place:** FUNDACION PRIVADA INSTITUT CATALA DE NANOTECNOLOGIA

**City of entity:** Barcelona, Catalonia, Spain



**Name principal investigator (PI, Co-PI....):** Pablo Ordejón Rontomé; Miguel Alonso Pruneda; Alberto García; Ramón Cuadrado del Burgo

**Nº of researchers:** 3

**Start-End date:** 15/06/2015 - 30/06/2016

**Applicant's contribution:** During the time of this project at the ICN2, I was in charge of the implementation and testing the on-site and the off-site Spin-Orbit Coupling (SOC) approximation within the official SIESTA DFT code. In doing so, I had to adapt the underlying SOC mathematical formalism to the current new MPI libraries of SIESTA. New tests and a specific manual entry was written regarding the implementation.

**3 Name of the project:** Femtospin

**Entity where project took place:** The University of York **Type of entity:** University

**City of entity:** York, North Yorkshire, United Kingdom

**Name principal investigator (PI, Co-PI....):** Roy William Chantrell

**Nº of researchers:** 20

**Start-End date:** 2012 - 2015

**4 Name of the project:** Physics of the optomagnetic reversal mechanism in which the magnetisation of magnetic material can be switched using circularly polarised laser light

**Entity where project took place:** The University of York **Type of entity:** University

**City of entity:** York, North Yorkshire, United Kingdom

**Name principal investigator (PI, Co-PI....):** Roy William Chantrell; Richard F. L. Evans; Ramón Cuadrado del Burgo; Thomas Andrew Ostler

**Nº of researchers:** 4

**Start-End date:** 2009 - 2012

**Applicant's contribution:** My duties as a sole member in R. Chantrell's group expert in ab initio modelization I was involved in several industrial and research projects with Samsung, Seagate and Toyota. I was focused in the achievement of geometrical ground state of different thin films and nanoparticles based on FePt-L1<sub>0</sub> alloys. In addition, their electronic and magnetic structure was studied by means of DFT calculations with SIESTA.

**5 Name of the project:** Dinámica y Electrónica de Espín en Nanomateriales: Estructuras Epitaxiales Crecidas por MBE y Modelización

**Entity where project took place:** Instituto de Ciencia de Materiales de Madrid **Type of entity:** State agency

**City of entity:** Madrid, Community of Madrid, Spain

**Name principal investigator (PI, Co-PI....):** Jorge Iribas Cerdá

**Nº of researchers:** 10

**Start-End date:** 2007 - 2011

**Applicant's contribution:** The aim of the applicant in this project was to unveil geometric, electronic and magnetic properties of different kind of magnetic and non-magnetic systems such as nanoparticles in gas phases, multilayered compounds and supported molecules on surfaces. The steps followed by the student were firstly the fabrication of different thicknesses and types of thin films by means of Pulse Laser Deposition (PLD) technique. Next, it was performed the geometrical characterisation using X-ray diffractometer and subsequent measure of the magnetic properties with the Vibrating Sample Magnetometer (VSM). Finally to model the material using cutting-edge computational quantum mechanical models. The successful application of all these process (mainly in its modelling stage) led to the doctorate achievement in 2011 entitled: "Simulación de propiedades electrónicas y magnéticas de sistemas mesoscópicos".

**6 Name of the project:** Magnetic Films for MEMS Applications

**Entity where project took place:** Instituto de Magnetismo Aplicado **Type of entity:** R&D Centre

**City of entity:** Madrid, Community of Madrid, Spain



**Name principal investigator (PI, Co-PI....):** Jesús María González Fernández  
**Nº of researchers:** 10  
**Start-End date:** 2004 - 2005

- 7** **Name of the project:** Nanoestructuras magnéticas de relevancia en dispositivos: crecimiento, efectos de intercara, propiedades y modelización  
**Entity where project took place:** Instituto de Ciencia de Materiales de Madrid  
**Type of entity:** State agency  
**City of entity:** Madrid, Community of Madrid, Spain  
**Name principal investigator (PI, Co-PI....):** Javier Palomares Simón  
**Nº of researchers:** 10  
**Start-End date:** 2004 - 2005

### R&D non-competitive contracts, agreements or projects with public or private entities

- 1** **Name of the project:** Atomistic Simulation of Advanced Materials for MRAM applications  
**Degree of contribution:** Researcher  
**Name principal investigator (PI, Co-PI....):** Roy William Chantrell  
**Nº of researchers:** 5  
**Funding entity or bodies:** Samsung  
**Type of entity:** R&D Centre  
**City funding entity:** Los Angeles, United States of America  
**Start date:** 01/02/2014  
**Duration:** 3 years
- 2** **Name of the project:** MagHEM  
**Degree of contribution:** Researcher  
**Name principal investigator (PI, Co-PI....):** Roy William Chantrell  
**Nº of researchers:** 10  
**Funding entity or bodies:** Toyota Motor Corporation  
**Type of entity:** R&D Centre  
**City funding entity:** Tokyo, Japan  
**Start date:** 01/06/2012  
**Duration:** 3 years



## Scientific and technological activities

### Scientific production

#### Publications, scientific and technical documents

- 1 Ramón Cuadrado; Miguel Alonso Pruneda; Alberto García; Pablo Ordejón. Implementation of non-collinear spin-constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian. *Journal of Physics: Materials*. 1, pp. 015010. 02/11/2018.  
**Type of production:** Scientific paper
- 2 Ramón Cuadrado; László Oroszlány; András Deák; Thomas A. Ostler; Andrea Meo; Roman V. Chepulsii; Dmytro Apalkov; Richard F. L. Evans; László Szunyogh; Roy W. Chantrell. Site-Resolved Contributions to the Magnetic-Anisotropy Energy and Complex Spin Structure of Fe/MgO Sandwiches. *Physical Review Applied*. 9, pp. 054048. 30/05/2018.  
**Type of production:** Scientific paper
- 3 Ramón Cuadrado; László Oroszlány; László Szunyogh; Gino Hrkac; Roy W. Chantrell; Thomas A. Ostler. A multiscale model of the effect of Ir thickness on the static and dynamic properties of Fe/Ir/Fe films. *Scientific Reports*. 8, pp. 3879. 01/03/2018.  
**Type of production:** Scientific paper
- 4 Pierluigi Gargiani; Ramón Cuadrado; Hari Babu Vasili; Miguel Alonso Pruneda; Manuel Valvidares. Graphene-based synthetic antiferromagnets and ferrimagnets. *Nature Communications*. 8, pp. 699. 26/09/2017.  
**Type of production:** Scientific paper
- 5 Jay Chureemart; Ramón Cuadrado; Panwade Chureemart; Roy W. Chantrell. Multiscale modeling of spin transport across a diffuse interface. *Journal of Magnetism and Magnetic Materials*. 443, pp. 287. 25/07/2017.  
**Type of production:** Scientific paper
- 6 Alberto Quintana; Jin Zhang; Eloy Isarain-Chávez; Enric Menéndez; Ramón Cuadrado; Roberto Robles; Maria Dolors Baró; Miguel Guerrero; Salvador Pané; Bradley J. Nelson; Carlos Maria Müller; Pablo Ordejón; Josep Nogués; Eva Pellicer; Jordi Sort. Voltage-Induced Coercivity Reduction in Nanoporous Alloy Films: A Boost toward Energy-Efficient Magnetic Actuation. *Advanced Functional Materials*. 27 - 32, pp. 1701904. 13/07/2017.  
**Type of production:** Scientific paper
- 7 Ramón cuadrado del Burgo; Kai Liu; Timothy J. Klemmer; Roy W. Chantrell. In-plane/out-of-plane disorder influence on the magnetic anisotropy of Fe<sub>1-y</sub>Mn<sub>y</sub>Pt-L1<sub>0</sub> bulk alloy. *Applied Physics Letters*. 108, pp. 123102. 21/03/2016.  
**Type of production:** Scientific paper
- 8 Thomas Bose; Ramón Cuadrado; Richard F. L. Evans; Roman V. Chepulsii; Dmytro Apalkov; Roy W. Chantrell. First-principles study of the Fe|MgO(001) interface: magnetic anisotropy. *Journal of Physics: Condensed Matter*. 28, pp. 156003. 17/03/2016.  
**Type of production:** Scientific paper
- 9 Thomas A. Ostler; Ramon Cuadrado; Roy Chantrell; Andrew W. Rushforth; Stuart A. Cavill. Strain Induced Vortex Core Switching in Planar Magnetostrictive Nanostructures. *Physical Review Letters*. 115, pp. 067202. 07/08/2015.  
**Type of production:** Scientific paper  
**Format:** Journal



- 10** Ramon Cuadrado; Roy Chantrell. Interaction potential of FePt with the MgO(001) surface. *Physical Review B*. 91, pp. 075420. 19/02/2015.  
**Type of production:** Scientific paper **Format:** Journal
- 11** Ramón Cuadrado del Burgo; Timothy J. Klemmer; Roy William Chantrell. Magnetic anisotropy of Fe<sub>1-y</sub>X<sub>y</sub>Pt – L1<sub>0</sub> [X=Cr,Mn,Co,Ni,Cu] bulk alloys. *Applied Physics Letters*. 105, pp. 152406-1 - 152406-4. 15/10/2014.  
**Type of production:** Scientific paper **Format:** Journal
- 12** Ramón Cuadrado del Burgo; Roy William Chantrell. Interface magnetic moments enhancement of FePt L1<sub>0</sub>/MgO(001): an ab-initio study. *Physical Review B*. 89, pp. 094407-1 - 094407-7. 07/03/2014.  
**Type of production:** Scientific paper **Format:** Journal
- 13** Cecilia Aas; Phil Hasnip; Ramón Cuadrado del Burgo; Ekaterina Plotnikova; Laszlo Szunyog; Laszlo Udvardi; Roy William Chantrell. Exchange coupling and magnetic anisotropy at Fe/FePt interfaces. *Physical Review B*. 88, pp. 174409-1 - 174409-11. 13/11/2013.  
**Type of production:** Scientific paper **Format:** Journal
- 14** Ramón Cuadrado del Burgo; Juan Manuel Puerta; Federico Soria; Jorge Iribas Cerdá. A first principles study of thiol-capped Au nanoparticles: Structural, electronic, and magnetic properties as a function of thiol coverage. *The Journal of Chemical Physics*. 139, pp. 034319-1 - 034319-10. 19/07/2013.  
**Type of production:** Scientific paper **Format:** Journal
- 15** Phanwadee Chureemart; Ramón Cuadrado del Burgo; Irene D'Amico; Roy William Chantrell. Modeling spin injection across diffuse interfaces. *Physical Review B*. 87, pp. 195310-1 - 195310-6. 21/05/2013.  
**Type of production:** Scientific paper **Format:** Journal
- 16** Ramón Cuadrado del Burgo; Roy William Chantrell. Electronic and magnetic properties of bimetallic L1<sub>0</sub> cuboctahedral clusters by means of a fully relativistic density functional based calculations. *Physical Review B*. 86, pp. 224415-1 - 224415-9. 18/12/2012.  
**Type of production:** Scientific paper **Format:** Journal
- 17** Ramón Cuadrado del Burgo; Jorge Iribas Cerdá. Fully relativistic pseudopotential formalism under an atomic orbital basis: spin–orbit splittings and magnetic anisotropies. *Journal of Physics: Condensed Matter*. 24, pp. 086005-1 - 086005-15. 26/01/2012.  
**Type of production:** Scientific paper **Format:** Journal
- 18** Ramón Cuadrado del Burgo; Jorge Iribas Cerdá; Yongfeng Wang; Ge Xin; Richard Berndt; Hao Tang. CoPc adsorption on Cu(111): origin of the C<sub>4</sub> to C<sub>2</sub> symmetry reduction. *The Journal of Chemical Physics*. 133, pp. 154701-1 - 154701-7. 15/10/2010.  
**Type of production:** Scientific paper **Format:** Journal
- 19** Ricardo Rurali; Ramón Cuadrado del Burgo; Jorge Iribas. C<sub>60</sub> adsorption on the Si(111)-p(7x7) surface: A theoretical study. *Physical Review B*. 81, pp. 075419-1 - 075419-9. 17/02/2010.  
**Type of production:** Scientific paper **Format:** Journal
- 20** Alfonso Rebolledo; Juan José Romero; Ramón Cuadrado del Burgo; Jesús María González; Fernando Pigazo; Francisco Javier Palomares; Miguel H. Medina; Guillermo Perez-Alcázar. Polymer bonded anisotropic thick hard films for micromotors/microgenerators. *Journal of Magnetism and Magnetic Materials* 316 (2007) e418–e421. 316, pp. e418 - e421. 02/03/2007.  
**Type of production:** Scientific paper **Format:** Journal





- 21** Juan José Romero; Ramón Cuadrado del Burgo; Elena Pina; Alfonso de Hoyos; Fernando Pigazo; Francisco Javier Palomares; Antonio Hernando; Roberto Sastre; Jesús María González. Anisotropic polymer bonded hard-magnetic films for microelectromechanical system applications. Journal of Applied Physics. 99, pp. 08N303-1 - 08N303-3. 26/04/2006.  
**Type of production:** Scientific paper **Format:** Journal
- 22** Francisco Javier Palomares; Fernando Pigazo; Juan José Romero; Ramón Cuadrado del Burgo; Alfredo Arroyo; Miguel Angel Gracia; Antonio Hernando; Raquel Cortés-Gil; José M. González-Calbet; María Vallet-Regí; Jesús María González; José M. Alonso. Temperature dependence of the magnetic properties in LaMnO<sub>3</sub> + delta. Journal of Applied Physics. 99, pp. 808A702-1 - 808A702-3. 18/04/2006.  
**Type of production:** Scientific paper **Format:** Journal
- 23** Juan José Romero; Francisco Javier Palomares; Fernando Pigazo; Ramón Cuadrado del Burgo; Federico Cebollada; Antonio Hernando; Jesús María González. Crystallization and magnetic hardening of SmCo thin films. Journal of Non-Crystalline Solids. 353, pp. 786 - 789. 09/02/2006.  
**Type of production:** Scientific paper **Format:** Journal
- 24** Juan José Romero; Francisco Javier Palomares; Fernando Pigazo; Ramón Cuadrado del Burgo; Roberto Sastre; Federico Cebollada; Antonio Hernando; Jesús María González. Polymer bonded anisotropic thick hard films for micromotors/microgenerators. Journal of iron and steel research international. 13, pp. 240 - 251. 2006.  
**Type of production:** Scientific paper **Format:** Journal

### Works submitted to national or international conferences

- 1** **Title of the work:** Implementation of non-collinear spin- constrained DFT calculations in SIESTA with a fully relativistic Hamiltonian  
**Name of the conference:** 19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods 2019  
**Type of participation:** 'Participatory - poster  
**City of event:** Trieste, Italy  
**Date of event:** 01/2019
- 2** **Title of the work:** pin-Orbit implementation by means of fully separable Kleinman-Bylander pseudopotential formalism under atomic orbital basis in SIESTA code  
**Name of the conference:** MAX International Conference 2018  
**Type of participation:** 'Participatory - poster  
**City of event:** Trieste, Italy  
**Date of event:** 01/2018  
Ramón Cuadrado; Jorge Iribas Cerdá; Miguel Alonso Pruneda; Alberto García; Pablo Ordejón.
- 3** **Title of the work:** Graphene-based synthetic antiferromagnets: an ab-initio study  
**Name of the conference:** 18th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods 2017  
**Type of participation:** 'Participatory - poster  
**City of event:** Trieste, Italy  
**Date of event:** 01/2017  
Ramón Cuadrado; Miguel Alonso Pruneda; Pablo Ordejón.
- 4** **Title of the work:** Atomistic spin dynamics and temperature dependent properties of Nd<sub>2</sub>Fe<sub>14</sub>B  
**Name of the conference:** Joint MMM/Intermag Conference 2016  
**Type of participation:** Participatory - oral communication



**City of event:** San Diego, United States of America

**Date of event:** 11/2016

Richard F. L. Evans; Ramón Cuadrado; Roy W. Chantrell.

- 5** **Title of the work:** Site-resolved contributions to the magnetic anisotropy energy and sperrimagnetic nature of Fe/MgO sandwiches  
**Name of the conference:** Joint MMM/Intermag Conference 2016  
**Type of participation:** 'Participatory - poster  
**City of event:** San Diego, United States of America  
**Date of event:** 11/2016  
Ramón Cuadrado; Thomas Ostler; Richard F. L. Evans; Andrea Meo; László Szunyogh; Roy W. Chantrell.
- 6** **Title of the work:** Magnetic anisotropy of Fe<sub>1-y</sub>X<sub>y</sub>Pt-L1<sub>0</sub> [X=Cr,Mn,Co,Ni,Cu] bulk alloys  
**Name of the conference:** ICM 2015  
**Type of participation:** 'Participatory - poster  
**City of event:** Barcelona, Catalonia, Spain  
**Date of event:** 05/07/2015  
Ramón Cuadrado del Burgo; Timothy J. Klemmer; Roy William Chantrell. "Magnetic anisotropy of Fe<sub>1-y</sub>X<sub>y</sub>Pt-L1<sub>0</sub> [X=Cr,Mn,Co,Ni,Cu] bulk alloys".
- 7** **Title of the work:** Strain Induced Vortex Core Switching in Planar Magnetostrictive Nanostructures  
**Name of the conference:** INTERMAG 2015  
**Type of participation:** Participatory - oral communication  
**City of event:** Beijing, China  
**Date of event:** 11/05/2015  
Thomas Andrew Ostler; Ramón Cuadrado del Burgo; Roy William Chantrell; A. W. Rushforth; Stuart A. Cavill.
- 8** **Title of the work:** Magnetic anisotropy of Fe<sub>1-y</sub>X<sub>y</sub>Pt-L1<sub>0</sub> [X=Cr,Mn,Co,Ni,Cu] bulk alloys  
**Name of the conference:** MAGNETISM 2015  
**Type of participation:** 'Participatory - poster  
**City of event:** LEEDS, United Kingdom  
**Date of event:** 30/03/2015  
Ramón Cuadrado del Burgo; Timothy J. Klemmer; Roy William Chantrell.
- 9** **Title of the work:** Strain Induced Vortex Core Switching in Planar Magnetostrictive Nanostructures  
**Name of the conference:** MAGNETISM 2015  
**Type of participation:** Participatory - oral communication  
**City of event:** Beijing, United Kingdom  
**Date of event:** 30/03/2015  
Thomas Andrew Ostler; Ramón Cuadrado del Burgo; Roy William Chantrell; A. W. Rushforth; Stuart A. Cavill.
- 10** **Title of the work:** Multiscale modeling: Atomistic spin models with ab-initio parametrisation  
**Name of the conference:** INTERMAG 2014  
**Type of participation:** Participatory - oral communication  
**City of event:** Dresden, Germany  
**Date of event:** 04/05/2014  
Richard F.L. Evans; Ramón Cuadrado del Burgo; Roy William Chantrell.



- 11 Title of the work:** Spin transport across the diffuse interface via multiscale calculation  
**Name of the conference:** INTERMAG 2014  
**Type of participation:** Participatory - oral communication  
**City of event:** Dresden, Germany  
**Date of event:** 04/05/2014  
Phanwadee Chureemart; Ramón Cuadrado del Burgo; Roy William Chantrell.
- 12 Title of the work:** Electronic and magnetic properties of bimetallic L1<sub>0</sub> cuboctahedral clusters by means of fully relativistic density-functional-based calculations  
**Name of the conference:** MAGNETISM 2014  
**Type of participation:** Participatory - oral communication  
**City of event:** Manchester, United Kingdom  
**Date of event:** 07/04/2014  
Ramón Cuadrado del Burgo; Roy William Chantrell.
- 13 Title of the work:** Atomistic modelling of temperature dependent properties of NdFeB  
**Name of the conference:** Magnetism and Magnetic Materials 2013  
**Type of participation:** Participatory - oral communication  
**City of event:** Denver, United States of America  
**Date of event:** 04/11/2013  
Richard F.L. Evans; Ramón Cuadrado; Roy William Chantrell.
- 14 Title of the work:** Exchange coupling and magnetic anisotropy at Fe/FePt interfaces  
**Name of the conference:** Magnetism and Magnetic Materials 2013  
**Type of participation:** Participatory - oral communication  
**City of event:** Denver, United States of America  
**Date of event:** 04/11/2013  
Cecilia Aas; Phil Hasnip; Ramón Cuadrado; Ekaterina Plotnikova; Laszlo Szunyog; Laszlo Udvardi; Roy William Chantrell.
- 15 Title of the work:** A model of spin injection including the effect of interface diffusion  
**Name of the conference:** The 12th Joint MMM/INTERMAG Conference  
**Type of participation:** Participatory - oral communication  
**City of event:** Chicago, United States of America  
**Date of event:** 13/01/2013  
Phanwadee Chureemart; Ramón Cuadrado del Burgo; Irene D'amico; Roy Chantrell.
- 16 Title of the work:** Magnetic anisotropy of L1<sub>0</sub> cuboctahedral nanoparticles by means of relativistic density functional calculations  
**Name of the conference:** Joint European magnetic symposia 2012  
**Type of participation:** Participatory - poster  
**City of event:** Parma, Italy  
**Date of event:** 12/09/2012  
Ramón Cuadrado del Burgo; Roy William Chantrell.
- 17 Title of the work:** Fully relativistic pseudopotential formalism under an atomic orbital basis: magnetic anisotropies  
**Name of the conference:** York-Tohoku Research Symposium 2011  
**Type of participation:** Participatory - poster  
**City of event:** York, United Kingdom  
**Date of event:** 11/06/2011



Ramón Cuadrado del Burgo; Roy William Chantrell; Jorge Iribas Cerdá.

- 18** **Title of the work:** CoPc adsorption on Cu(111): origin of the C4 to C2 symmetry reduction  
**Name of the conference:** Fuerzas y Tunel 2010  
**Type of participation:** Participatory - oral communication  
**City of event:** Tarragona, Spain  
**Date of event:** 10/09/2010  
Hao Tang; Ramón Cuadrado del Burgo; Jorge Iribas Cerdá; Yongfeng Wang; Ge Xin; Richard Berndt.
- 19** **Title of the work:** A first principles study of thiol-capped Au Nanoparticles: structural and electronic properties as a function of thiol coverages  
**Name of the conference:** GEFES 2010  
**Type of participation:** Participatory - poster  
**City of event:** Zaragoza, Spain  
**Date of event:** 10/02/2010  
Ramón Cuadrado del Burgo; Jorge Iribas Cerdá.
- 20** **Title of the work:** A first principles study of thiol-capped Au Nanoparticles  
**Name of the conference:** INTERMAG 2008  
**Type of participation:** Participatory - poster  
**City of event:** Madrid, Spain  
**Date of event:** 08/05/2008  
Ramón Cuadrado del Burgo; Jorge Iribas Cerdá.
- 21** **Title of the work:** Anisotropic polymer bonded hard-magnetic films for MEMS applications  
**Name of the conference:** Magnetism and Magnetic Materials 2005  
**Type of participation:** Participatory - oral communication  
**City of event:** San Diego, United States of America  
**Date of event:** 05/11/2005  
Júan José Romero; Ramón Cuadrado del Burgo; Elena Pina; Alfonso de Hoyos; Fernando Pigazo; Francisco Javier Palomares; Antonio Hernando; Roberto Sastre; Jesús María González-Fernández.
- 22** **Title of the work:** Temperature dependence of the hysteretic properties in LaMnO<sub>3</sub>+<sub>delta</sub>  
**Name of the conference:** Magnetism and Magnetic Materials 2005  
**Type of participation:** Participatory - oral communication  
**City of event:** San Diego, United States of America  
**Date of event:** 05/11/2005  
Francisco Javier Palomares; Fernando Pigazo; Júan José Romero; Ramón Cuadrado del Burgo; Alfredo Arroyo; Miguel Angel García; Antonio Hernando; Raquel Cortés-Gil; José María González-Calbet; María Vallet-Regí.
- 23** **Title of the work:** Temperature dependence of the hysteretic properties in LaMnO<sub>3</sub>+<sub>delta</sub>  
**Name of the conference:** INTERMAG 2005  
**Type of participation:** Participatory - oral communication  
**City of event:** Nagoya, Japan  
**Date of event:** 05/04/2005  
Francisco Javier Palomares; Fernando Pigazo; Júan José Romero; Ramón Cuadrado del Burgo; Alfredo Arroyo; Miguel Angel García; Antonio Hernando; Raquel Cortés-Gil; José María González-Calbet; María Vallet-Regí.



## R&D management and participation in scientific committees

### Organization of R&D activities

- 1** **Title of the activity:** Magnetism Open Knowledge Workshop  
**Type of activity:** Workshop **Geographical area:** National  
**Convening entity:** Instituto Catalan de Nanociencia y Nanotecnología (ICN2)  
**City convening entity:** Barcelona, Catalonia, Spain  
**Type of participation:** Organiser  
**Nº assistants:** 12  
**Start-End date:** 20/06/2018 - 22/06/2018 **Duration:** 3 days
- 2** **Title of the activity:** SIESTA School at Barcelona Supercomputer Center (BSC)  
**Type of activity:** School **Geographical area:** National  
**Convening entity:** Barcelona Supercomputer Center (BSC)  
**City convening entity:** Barcelona, Catalonia, Spain  
**Type of participation:** Organiser  
**Nº assistants:** 20  
**Start-End date:** 08/05/2017 - 11/05/2017 **Duration:** 4 days
- 3** **Title of the activity:** INTERMAG 2014  
**Type of activity:** Chairman at INTERMAG Dresden, **Geographical area:** Non EU International  
Germany  
**City convening entity:** Dresden, Germany  
**Start-End date:** 05/05/2014 - 05/11/2014 **Duration:** 1 day

### Evaluation and revision of R&D projects and articles

- 1** **Name of the activity:** Referee of Journal of Physics: Materials  
**Performed tasks:** Referee of Journal of Physics: Materials  
**City of entity:** Barcelona, Catalonia, Spain  
**Geographical area:** Non EU International  
**Start date:** 2017
- 2** **Name of the activity:** Referee of international Journals  
**Performed tasks:** Referee of Applied Physics Letters  
**City of entity:** York, United Kingdom  
**Start date:** 2012
- 3** **Name of the activity:** Referee of international Journals  
**Performed tasks:** Referee of Journal of Magnetism and Magnetic Materials  
**City of entity:** York, United Kingdom  
**Start date:** 2012
- 4** **Name of the activity:** Referee of international Journals  
**Performed tasks:** Referee of Physical Review Letters  
**City of entity:** York, United Kingdom



**Start date:** 2012

- 5 Name of the activity:** Referee of Physical Review B  
**Performed tasks:** Referee of Physical review B  
**City of entity:** York, United Kingdom  
**Start date:** 2012

## Other achievements

### Stays in public or private R&D centres

**Entity:** Toyota Motor Corporation  
**City of entity:** Tokyo, Japan  
**Start date:** 09/2014  
**Goals of the stay:** Post-doctoral  
**Provable tasks:** Invited talk  
**Type of entity:** R&D Centre  
**Duration:** 7 days

### Obtained grants and scholarships

- 1 Name of the grant:** Marie Sklodowska-Curie Incoming (COFUND) Fellow  
**Aims:** Post-doctoral  
**Awarding entity:** Universidad Autónoma de Barcelona - European Union FP7  
**Conferral date:** 01/07/2016  
**Duration:** 3 years  
**End date:** 30/06/2019  
**Entity where activity was carried out:** Universitat Autònoma de Barcelona  
**Faculty, institute or centre:** ICN2
- 2 Name of the grant:** Marie Curie Institutional Fellowship  
**Aims:** Post-doctoral  
**Awarding entity:** The University of York  
**Conferral date:** 05/2011  
**Duration:** 2 years  
**End date:** 04/2013  
**Entity where activity was carried out:** The University of York  
**Faculty, institute or centre:** Physics
- 3 Name of the grant:** Formación Personal Investigador (FPI)  
**Aims:** Pre-doctoral  
**Awarding entity:** Ministerio de Ciencia e Innovación  
**Type of entity:** Pública  
**Conferral date:** 08/2006  
**Duration:** 4 years  
**End date:** 08/2010  
**Entity where activity was carried out:** Instituto de Ciencia de Materiales de Madrid