CURRÍCULUM VÍTAE NORMALIZADO

ALEJANDRO GAITA ARIÑO

Generated from: Editor CVN de FECYT

Date of document: 03/10/2017

v 1.4.0

0af74c85a8d70b0e3b3f3807fe5a78f3

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.

My two current main research interests are **spin qubits** and **rare-earth single-ion magnets**. In each one of these two fields I have made seminal contributions which have strongly impacted in the molecular magnetism community. The first one concerns the proposal of using molecular systems for the coupling of two spin qubits in order to develop a quantum gate (published in Nature Nanotechnology. 2007); this theoretical work had a strong impact in the nascent field of molecular spintronics since it proposed the way of controling the spin state of a molecular system through an electrical current. The second was the discovery that lanthanoid mononuclear complexes based on polyoxometalates behave as single-molecule magnets (published in JACS, 2008). This work showed to the chemists working in molecular magnetism the key role played by the crystal field around the lanthanide in the magnetic properties exhibited by these mononuclear complexes, which represent the ultimate step towards the miniaturisation of the single-molecule magnets, as a single metal ion, rather than a magnetic cluster, is enough to behave as a tiny magnet. The combination of the two fields resulted in the design of a polyoxometalate spin qubit presenting atomic clock transition (published in Nature, 2016).

For both fields, these contributions were the first published papers about these topics at the ICMol, hence, they served to open two new lines of research. Nowadays a total of around 30 researchers and technicians are working at the ICMol in these two lines. This research line has been reinforced since **I was awarded a ERC Consolidator Grant (2015-2020)** entitled **"A chemical approach to molecular spin qubits: decoherence and organisation of rare earth single ion magnets.".**

Four PhD students have been working in these lines of research under my supervision since then: M. A. AlDamen, S. Cardona-Serra, J. J. Baldoví and L. Escalera (M.A.A. is now Distinguished Researcher in the U. of Jordan, has obtained funding and supervises a PhD working in the same topic., J.J.B. just started a Marie Curie postdoctoral fellowship). Moreover, my theoretical team is a reference for molecular spin qubits in Spain, being the only Chemistry team regularly participating in the Workshops on Quantum Information in Spain since their inception (2012).

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.

Over 50 scientific publications in 1st quartile international journals, including:
1x Nature 1x Nature Nanotechnology 2x Phys. Rev. Lett.
1x Angew. Chem. Int. Ed. 1x Chem. Soc. Rev. 3x J. Am. Chem. Soc.
2x J. Phys. Chem. Lett. 2x Chem. Commun. 1x Chem. Sci.
6x Chem. Eur. J. 2x J. Mater. Chem. 7x Inorg. Chem.
3x Inorg. Chem. Front. 2x Dalton Trans. 2x J. Comput. Chem.

-Corresponding Author in 14 publications
 # cit.:2720(>25% since 2016) ; **# cit./year [2012-2016]:383 ; h -index = 25 ; cit./article = 45**

ALEJANDRO GAITA ARIÑO

Surname(s): **GAITA ARIÑO**
Name: **ALEJANDRO**
DNI: **44852423P**
Date of birth: **26/05/1976**
Gender: **Male**
Land line phone: **963544421 - 4418**
Email: **Alejandro.Gaita@uv.es**

Current professional situation

Employing entity: Universitat de València **Type of entity:** University
Department: Instituto de Ciencia Molecular
Professional category: Senior postdoc, Ramón y Cajal
Start date: 01/11/2013
Type of contract: Temporary employment contract

Previous positions and activities

	Employing entity	Professional category	Start date
1	Universitat de València	Superior Research Technician	01/09/2011
2	Universitat de València	Postdoctoral Fellow contract, paid by the EU - VIII FP	01/09/2010
3	PITP / UBC	Postdoctoral Fellow contract, paid by the EU - VIII FP	01/09/2008
4	PITP / UBC	Postdoctoral Fellow contract, paid by the Ministerio de Innovacion y cultura	01/09/2007
5	Instituto de Ciencia Molecular / UVEG	Postdoctoral Fellow contract, paid by the Generalitat Valenciana	01/07/2007
6	Instituto de Ciencia Molecular / UVEG	Superior Research Technician	01/08/2004
7	Instituto de Ciencia Molecular / UVEG	Collaboration grant	01/01/2004
8	Departamento de Química Inorgánica e ICMol / UVEG	PhD grant	01/01/2000
9	Departamento de Química Inorgánica / UVEG	Collaboration grant	01/09/1998

1 **Employing entity:** Universitat de València **Type of entity:** University
Professional category: Superior Research Technician
Start-End date: 01/09/2011 - 31/10/2013

2 **Employing entity:** Universitat de València
Professional category: Postdoctoral Fellow contract, paid by the EU - VIII FP
Start date: 01/09/2010 **Duration:** 1 year

3 **Employing entity:** PITP / UBC
Professional category: Postdoctoral Fellow contract, paid by the EU - VIII FP
Start date: 01/09/2008 **Duration:** 2 years

4 **Employing entity:** PITP / UBC
Professional category: Postdoctoral Fellow contract, paid by the Ministerio de Innovacion y cultura
Start date: 01/09/2007 **Duration:** 1 year

5 **Employing entity:** Instituto de Ciencia Molecular / UVEG
Professional category: Postdoctoral Fellow contract, paid by the Generalitat Valenciana
Start date: 01/07/2007 **Duration:** 2 months

6 **Employing entity:** Instituto de Ciencia Molecular / UVEG
Professional category: Superior Research Technician
Start date: 01/08/2004 **Duration:** 2 years - 11 months

7 **Employing entity:** Instituto de Ciencia Molecular / UVEG
Professional category: Collaboration grant
Start date: 01/01/2004 **Duration:** 6 months

8 **Employing entity:** Departamento de Química Inorgánica e ICMol / UVEG
Professional category: PhD grant
Start date: 01/01/2000 **Duration:** 4 years

9 **Employing entity:** Departamento de Química Inorgánica / UVEG
Professional category: Collaboration grant
Start date: 01/09/1998 **Duration:** 1 year

Education

University education

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

University degree: Diplomatura / Licenciatura / Grado
Name of qualification: Licenciado en Química
Degree awarding entity: Universitat de València
Date of qualification: 23/08/1999

Doctorates

Doctorate programme: Doctor en Química
Degree awarding entity: Universitat de València
Date of degree: 27/07/2004
Thesis title: Interacciones magnéticas y deslocalización electrónica en materiales moleculares
Thesis director: Eugenio Coronado Miralles y Juan Modesto Clemente Juan
Obtained qualification: Sobresaliente cum laude

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
French	B1	B1	A1	A1	A1
German	B1	B1	B1	B1	A1
Catalan	B1	C1	B1	B1	B1
Esperanto	B1	C1	B1	B1	B1
English	C1	C2	C1	C1	C1
Spanish	C2	C2	C2	C2	C2

Teaching experience

Experience supervising doctoral thesis and/or final year projects

1 **Project title:** Development of computational code for the study off single ion magnets and molecular spin qubits
Type of project: Work leading to an ASD
Co-director of thesis: A. Gaita-Ariño; S. Cardona-Serra; J. J. Baldoví
Entity: Université Paul Savatier **Type of entity:** University
City of entity: Toulouse, France
Student: A. Schahl
Date of reading: 23/06/2016
Date of award: 23/06/2016

2 **Project title:** Rational design and modelling of f-block molecular nanomagnets
Type of project: Doctoral thesis
Entity: Universitat de València **Type of entity:** University
Student: José J. Baldoví
Obtained qualification: Excellent cum laude
Date of reading: 2016

3 **Project title:** Theoretical studies on decoherence processes in molecular spin qubits
Entity: Universitat de València **Type of entity:** University
Student: L. Escalera
Date of reading: 2015

4 **Project title:** Complejos de lantánidos con polioxometalatos
Type of project: Doctoral thesis
Entity: Universitat de València **Type of entity:** University
Student: Salvador Cardona Serra
Obtained qualification: Excellent cum laude
Date of reading: 2013

5 **Project title:** Development of a computational package for the rational design of SIMs and spin qubits
Type of project: Work leading to an ASD
Entity: Universitat de València **Type of entity:** University
Student: José Jaime Baldoví Jachán
Obtained qualification: Excellent
Date of reading: 2012

6 **Project title:** Complejos de lantánidos con polioxometalatos
Type of project: Work leading to an ASD
Entity: Universitat de València **Type of entity:** University
Student: Salvador Cardona Serra
Obtained qualification: Excellent
Date of reading: 2009

7 **Project title:** Theoretical Study of Polyoxometalates with Interest in Molecular Magnetism
Type of project: Doctoral thesis
Entity: Universitat de València
Student: Murad Abbas Abdallah AlDamen
Obtained qualification: Excellent cum laude
Date of reading: 2008

8 **Project title:** Interacciones Vibrónicas en compuestos de Valencia Mixta
Type of project: End of course project
Entity: Universitat de València **Type of entity:** University
Student: Salvador Cardona Serra
Obtained qualification: Excellent
Date of reading: 2007

Scientific and technological experience

Scientific or technological activities

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

1 **Name of the project:** A Chemical Approach to Molecular Spin Qubits: Decoherence and Organisation of Rare Earth Single Ion Magnets
Type of project: Basic research (including archaeological digs, etc)
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universitat de València **Type of entity:** University
City of entity: Valencia, Valencian Community, Spain
Name principal investigator (PI, Co-PI....): A. Gaita-Ariño
Nº of researchers: 10
Funding entity or bodies:
European Research Council **Type of entity:** Public Research Body

Type of participation: Principal investigator
Start-End date: 01/08/2015 - 31/07/2020 **Duration:** 5 years
Total amount: 1.827.375 €
Applicant's contribution: I applied for (and was awarded) this ERC-CoG. Around 10 researchers are working / will be working with me on this project during these five years.

2 **Name of the project:** Moléculas magnéticas de interés en computación y espintrónica cuánticas
Entity where project took place: Universitat de València **Type of entity:** University
City of entity: Valencia, Valencian Community, Spain
Name principal investigator (PI, Co-PI....): J.M. Clemente-Juan; A. Gaita-Ariño
Start-End date: 01/11/2015 - 31/10/2018

3 **Name of the project:** Molspin (Molecular Spintronics)
Name principal investigator (PI, Co-PI....): E. Coronado; R. Sessoli; A. Dediu; H. van der Zant; F. Luis
Nº of researchers: 234
Funding entity or bodies:
European Union

Start date: 2015

4 **Name of the project:** DEL MAGNETISMO MOLECULAR A LA ESPINTRONICA MOLECULAR
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Funding entity or bodies:
Ministerio de Ciencia e Innovación

Start date: 2012
Total amount: 600.000,28 €

5 **Name of the project:** Electric Field Control Over Spin Molecules (ELFOS)
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): Eugenio Coronado Miralles
Nº of researchers: 8
Funding entity or bodies:
Comisión Europea **Type of entity:** Body, others

Start date: 2011
Total amount: 368.546 €

6 **Name of the project:** Next Generation Hybrid Interfaces for Spintronic Applications - HINTS
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): Eugenio Coronado Miralles
Nº of researchers: 14
Funding entity or bodies:
Unión Europea

Start date: 2011
Total amount: 293.600 €

7 **Name of the project:** Magnetic Molecules and Hybrid Materials for Molecular Spintronics, SPINMOL
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): Eugenio Coronado Miralles
Nº of researchers: 14
Funding entity or bodies:
European Research Council

Start date: 2010
Total amount: 1.679.700 €

8 **Name of the project:** Decoherence in magnetic molecules as qubits
Geographical area: Non EU International
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): Alejandro Gaita Ariño
Nº of researchers: 1
Funding entity or bodies:
European Union - Seventh Framework Programme

Code according to the funding entity: PIOF-GA-2008-219514
Start date: 2008 **Duration:** 3 years
Total amount: 220.373,32 €
Dedication regime: Full time

9 **Name of the project:** Materiales moleculares para el magnetismo y la electrónica molecular: del diseño, estudio y procesado de nuevos materiales al desarrollo de aplicaciones
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Nº of researchers: 15
Funding entity or bodies:
Ministerio de Educación y Ciencia. Dirección General de Investigación Científica y Técnica

Start date: 2007
Total amount: 1.243.880 €

10 **Name of the project:** Nanociencia molecular
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Nº of researchers: 108
Funding entity or bodies:
Ministerio de Educación y Ciencia. Dirección General de Investigación Científica y Técnica

Start date: 2007
Total amount: 5.750.000 €

11 **Name of the project:** REVIV: CIENCIA I TECNOLOGIA DE MATERIALS
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Funding entity or bodies:
Consellería de Empresa, Universidad y Ciencia- Generalitat Valenciana

Start date: 2007
Total amount: 12.000 €

12 **Name of the project:** Molecular Approach to Nanomagnets and Multifunctional Materials - MAGMANet
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Nº of researchers: 40
Funding entity or bodies:
Unión Europea

Start date: 2005
Total amount: 868.297 €

13 **Name of the project:** Magnetismo molecular: síntesis, caracterización y modelización de las propiedades físicas de clusters magnéticos y sistemas extendidos basados en la química de coordinación
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): C. Gómez
Nº of researchers: 5
Funding entity or bodies:
Generalitat Valenciana **Type of entity:** Body, others

Start date: 2004
Total amount: 15.000 €

14 **Name of the project:** AYUDA A GRUPOS 03/163
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Nº of researchers: 25
Funding entity or bodies:
Generalitat Valenciana **Type of entity:** Body, others

Start date: 2003
Total amount: 81.360,34 €

15 **Name of the project:** Unidad de investigación de materiales moleculares
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Funding entity or bodies:
Conselleria de Cultura Educació i esport

Start date: 2003
Total amount: 81.360,34 €

16 **Name of the project:** Ayudas a Actividades de I + D Cooperativas molecular approach to Nanomagnetic-Multifuncional Materials
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Funding entity or bodies:
Conselleria de Innovación y Competitividad, Gobierno Valenciano.

Start date: 2002

17 **Name of the project:** Clusters Magnéticos: Síntesis, propiedades y aplicaciones
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Nº of researchers: 6
Funding entity or bodies:
Generalitat Valenciana **Type of entity:** Body, others

Start date: 2002
Total amount: 18.000 €

18 **Name of the project:** Red temática de magnetismo molecular
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado
Funding entity or bodies:
Ministerio de Ciencia y Tecnología.

Start date: 2002

19 **Name of the project:** Low-dimensional conductors based on radical cation salts with photochromic and magnetic counter-ions: Synthesis, structure, optical, electrical and magnetic properties
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado (coordinador: E. Coronado)
Nº of researchers: 10
Funding entity or bodies:
International Association for the Promotion of Cooperation with scientists from the Independent States of the former Soviet Union (INTAS)

Start date: 2001
Total amount: 5.400 €

20 **Name of the project:** Materiales magnéticos moleculares: Materiales magnéticos multifuncionales y moléculas biestables para la electrónica molecular.
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): E. Coronado (coordinador: E. Coronado)
Nº of researchers: 15
Funding entity or bodies:

Ministerio de Ciencia y Tecnología, Dirección General de Investigación

Start date: 2001
Total amount: 222.374,49 €

21 **Name of the project:** Molecular nanomagnets.
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): Dante Gatteschi
Funding entity or bodies:
INTAS

Start date: 2000

22 **Name of the project:** Molecular Magnetism: from Materials to Devices.
Entity where project took place: Universitat de València
Name principal investigator (PI, Co-PI....): Miguel Julve (Coordinador: J. Veciana)
Funding entity or bodies:
Unió Europea

Start date: 1998
Total amount: 104.125,35 €

Scientific and technological activities

Scientific production

Publications, scientific and technical documents

1 M. Shiddiq; D. Komijani; Y. Duan; A. Gaita-Ariño; E. Coronado; S. Hill. Enhancing coherence in molecular spin qubits via atomic clock transitions. Nature. 531, pp. 348 - 351. 2016. ISSN 0028-0836
Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 58

Relevant publication: Yes

2 Juan M. Clemente-Juan; Eugenio Coronado; Alejandro Gaita-Ariño. Magnetic polyoxometalates: from molecular magnetism to molecular spintronics and quantum computing. Chemical Society Reviews. 41, pp. 7464 - 7478. (United Kingdom): 2012. ISSN 0306-0012
Type of production: Scientific paper **Format:** Journal

Impact source: Journal webpage
Impact index in year of publication: 28,76

Source of citations: WOS **Citations:** 274

Relevant publication: Yes

3 MA. AlDamen; S. Cardona-Serra; J.M. Clemente-Juan; E. Coronado; A. Gatia-Ariño; C. Martí-Gastaldo; F. Luis; O. Montero. Mononuclear Lanthanide Single-Molecule Magnets Based on Polyoxometalates . Inorganic Chemistry. 48, pp. 3467. (United States of America): 2009. ISSN 0020-1669
Type of production: Scientific paper **Format:** Journal
Impact source: SCI **Category:** CHEMISTRY, INORGANIC & NUCLEAR

Impact index in year of publication: 4,657 **Journal in the top 25%:** Yes
Position of publication: 3

Source of citations: WOS **Citations:** 284

Relevant results: 2th most cited paper of Inorganic Chemistry in 2009 (of a total of 1480); “highly cited paper” according to ISI Web of Knowledge.
Relevant publication: Yes

4 M.A. AlDamen; J.M. Clemente-Juan; E. Coronado; C. Marti-Gastaldo; A. Gaita-Ariño. Mononuclear Lanthanide Single-Molecular Magnets Based on Polyoxometalates. Journal of the American Chemical Society. 130, pp. 8874 - 8875. (United States of America): 2008. ISSN 0002-7863
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes

Impact source: SCI **Category:** CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 8,091 **Journal in the top 25%:** Yes
Position of publication: 7

Source of citations: WOS **Citations:** 499

Relevant results: In the top 40 cited papers of J. Am. Chem. Soc. in 2008 (of a total of 2951); “highly cited paper” according to ISI Web of Knowledge.
Relevant publication: Yes

5 J. Lehmann; A. Gaita-Ariño; E. Coronado; D. Loss. Spin qubits with electrically gated polyoxometalate molecules. Nature Nanotechnology. 23, pp. 312 - 317. (United Kingdom): 2007. ISSN 1748-3387
Type of production: Scientific paper **Format:** Journal

Impact source: SCI **Category:** NANOSCIENCE & NANOTECHNOLOGY
Impact index in year of publication: 14,917 **Journal in the top 25%:** Yes
Position of publication: 1

Source of citations: WOS **Citations:** 256

Relevant results: Cover of the journal, and highlighted by a “News and Views” article in the same issue.
Relevant publication: Yes

6 M.D. Jenkins; Y. Duan; B. Diosdado; J.J. García-Ripoll; A. Gaita-Ariño; C. Giménez-Saiz; P.J. Alonso; E. Coronado; F. Luis. Coherent manipulation of three-qubit states in a molecular single-ion magnet. Physical Review B. 95 - 6, pp. 064423. 2017. ISSN 2469-9950
Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 5

7 K. Soo Lim; J.J. Baldoví; S. Jiang; B. Ho Koo; D. Won Kang; W. Ram Lee; E. Kwan Koh; A. Gaita-Ariño; E. Coronado; M. Slota; L. Bogani; C. Seop Hong. Custom Coordination Environments for Lanthanoids: Tripodal Ligands Achieve Near-Perfect Octahedral Coordination for Two Dysprosium-Based Molecular Nanomagnets. Inorganic Chemistry. 2017. ISSN 0020-1669
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes

8 L. Escalera-Moreno; N. Suaud; A. Gaita-Ariño; E. Coronado. Determining Key Local Vibrations in the Relaxation of Molecular Spin Qubits and Single Molecule Magnets. Journal Of Physical Chemistry Letters. 8 - 7, pp. 1695 - 1700. American Chemical Society, 2017. ISSN 1948-7185
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 3

9 A. Palii; S. Aldoshin; B. Tsukerblat; J.M. Clemente-Juan; A. Gaita-Arino; E. Coronado. Electric field controllable magnetic coupling of localized spins mediated by itinerant electrons: a toy model.Physical chemistry chemical physics. Royal Society of Chemistry, 2017.
DOI: 10.1039/c7cp03872k
Type of production: Scientific paper

10 S. Cardona-Serra; A. Gaita-Arino; M. Stamenova; S. Sanvito. Theoretical Evaluation of [V-IV(alpha-C3S5)(3)](2-) as Nuclear-Spin-Sensitive Single-Molecule Spin Transistor. Journal Of Physical Chemistry Letters. 8 - 13, pp. 3056 - 3060. American Chemical Society, 2017.
Type of production: Scientific paper

11 A. Gaita-Ariño; H. Prima-García; S. Cardona-Serra; L. Escalera-Moreno; L. E. Rosaleny; J. J. Baldoví. Coherence and organisation in lanthanoid complexes: from single ion magnets to spin qubits. Inorganic Chemistry Frontiers. 3 - 5, pp. 568 - 577. 2016. ISSN 2052-1545
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 4

12 J.J. Baldoví; Y. Duan; R. Morales; A. Gaita-Ariño; E. Ruiz; E. Coronado. Rational Design of Lanthanoid Single-Ion Magnets: Predictive Power of the Theoretical Models.Chemistry-A European Journal. 22 - 38, pp. 13532 - 13539. 2016. ISSN 0947-6539
Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 5

13 S. Cardona-Serra; L. Escalera-Moreno; J.J. Baldoví; A. Gaita-Ariño; J.M. Clemente-Juan; E. Coronado. SIMPRE1. 2: Considering the hyperfine and quadrupolar couplings and the nuclear spin bath decoherence. Journal of Computational Chemistry. 37, pp. 1238 - 1244. 2016. Available on-line at: <http://pubs.rsc.org/en/content/articlelanding/2015/qi/c5qi00142k/unauth#!divAbstract>. ISSN 0192-8651
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 3

14 J. J. Baldoví; Y. Duan; C. Bustos; S. Cardona-Serra; P. Gouzerh; R. Villanneau; G. Gontard; J. M. Clemente Juan; A. Gaita-Ariño; C. Giménez-Saiz; A. Proust; E. Coronado. Single ion magnets based on lanthanoid Polyoxomolybdate complexes. Dalton Transactions. 45 - 42, pp. 16653 - 16660. 2016. Available on-line at: <http://pubs.rsc.org/EN/content/articlelanding/2016/dt/c6dt02258h#!divAbstract>. ISSN 1477-9226
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 2

15 K. Soo Lim; J.J. Baldoví; W. Ram Lee; J. Hwa Song; S. Won Yoon; B. Jin Suh; E. Coronado; A. Gaita-Ariño; C. Seop Hong. Switching of Slow Magnetic Relaxation Dynamics in Mononuclear Dysprosium (III) Compound with Charge Density. Inorganic Chemistry. 55, pp. 5398 - 5404. 2016. ISSN 0020-1669
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 3

16 L. E. Rosaleny; A. Gaita-Ariño. Theoretical evaluation of lanthanide binding tags as biomolecular handles for the organization of single ion magnets and spin qubits. Inorganic Chemistry Frontiers. 3, pp. 61 - 66. 2016. Available on-line at: <http://pubs.rsc.org/en/content/articlelanding/2016/qi/c5qi00127g/unauth#!divAbstract>. ISSN 2052-1545

Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 5

17 M.A. Antunes; J.T. Coutinho; I.C. Santos; J. Marçalo; L.C.J. Pereira; M. Almeida; J.J. Baldoví; E. Coronado; A. Gaita-Ariño. A Mononuclear Uranium(IV) Single-Molecule Magnet with an Azobenzene Radical Ligand. Chemistry-A European Journal. 21, pp. 17817 - 17826. 2015. ISSN 0947-6539

Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 6

18 K. Qian; J.J. Baldoví; S.-D. Jiang; A. Gaita-Ariño; Y.-Q. Zhang; J. Overgaard; B.-W. Wang; S. Gao E. Coronado. Does the thermal evolution of molecular structures critically affect the magnetic anisotropy?. Chemical Science. 6, pp. 4587 - 4593. 2015. ISSN 2041-6520

Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 22

19 S. Cardona-Serra; J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; N. Suaud; O. Svoboda; R. Bastardis; N. Guihery; J.J. Palacios. Electrically Switchable Magnetic Molecules: Inducing a Magnetic Coupling by Means of an External Electric Field in a Mixed- Valence Polyoxovanadate Cluster. Chemistry-A European Journal. 21 - 2, pp. 763 - 769. 2015. ISSN 0947-6539

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 10

20 V. F. González-Albuixech; A. Gaita-Ariño. Inexpensive discrete atomistic model technique for studying excitations on infinite disordered media: The case of orientational glass ArN2. International Journal for Numerical Methods in Engineering. 2015. ISSN 0029-5981

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

21 A. Gaita-Ariño; V. F. González-Albuixech; M. Schechter. Inversion symmetric vs. asymmetric excitations and the low-temperature universal properties of Ar:N2 and Ar:N2:CO glasses. Europhysics Letters. 109, pp. 56001. 2015. ISSN 0295-5075

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

22 B. Monteiro; J.T Coutinho; C.C.L. Pereira; L.C.J. Pereira; J. Marçalo; M. Almeida; J.J Baldoví; E. Coronado; A. Gaita-Ariño. Magnetic Properties of the Layered Lanthanide Hydroxide Series Y x Dy8-x (OH) 20Cl4· 6H2O: From Single Ion Magnets to 2D and 3D Interaction Effects. Inorganic Chemistry. 54, pp. 1949 - 1957. 2015. ISSN 0020-1669

Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 14

23 J.J. Baldoví; A. Gaita-Ariño; E. Coronado. Modeling the magnetic properties of lanthanide complexes: relationship of the REC parameters with Pauling electronegativity and coordination number. Dalton Transactions. 44, pp. 12535 - 12538. 2015. ISSN 1477-9226

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

Corresponding author: Yes
Source of citations: WOS **Citations:** 9

24 J.J. Baldoví; L.E. Rosaleny; V. Ramachandran; J. Christian; N.S. Dalal; J.M. Clemente-Juan; P. Yang; U. Kortz; A. Gaita-Ariño; E. Coronado. Molecular spin qubits based on lanthanide ions encapsulated in cubic polyoxopalladates: design criteria to enhance quantum coherence. Inorganic Chemistry Frontiers. 2, pp. 893 - 897. 2015. Available on-line at: <http://pubs.rsc.org/en/content/articlelanding/2015/qi/c5qi00142k/unauth#!divAbstract>. ISSN 2052-1545
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 4

25 J. J. Baldoví; S. Cardona-Serra; J. M. Clemente-Juan; L. Escalera-Moreno; A. Gaita-Ariño; G. Mínguez Espallargas.Quantum Error Correction with magnetic molecules. Europhysics Letters. 110, pp. 33001. 2015. ISSN 0295-5075
Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 4

26 J.J. Baldovi; E. Coronado; A. Gaita-Arino; C. Gamer; M. Gimenez-Marques; G. Minguez Espallargas. A SIM-MOF: Three-Dimensional Organisation of Single-Ion Magnets with Anion-Exchange Capabilities. Chemistry-A European Journal. 20 - 34, pp. 10695 - 10702. 2014. ISSN 0947-6539
Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 48

27 J.J. Baldoví; J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; A. Palii. An updated version of the computational package SIMPRE that uses the standard conventions for Stevens crystal field parameters. Journal of Computational Chemistry. 35 - 26, 2014. ISSN 0192-8651
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 15

28 J.J. Baldovi; J.M. Clemente-Juan; E. Coronado; Y. Duan; A. Gaita-Arino; C. Gimenez-Saiz. Construction of a General Library for the Rational Design of Nanomagnets and Spin Qubits Based on Mononuclear f-Block Complexes. The Polyoxometalate Case.Inorganic Chemistry. 53 - 18, pp. 9976 - 9980. 2014. ISSN 0020-1669
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes

29 J.J. Baldoví; J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño. Molecular Anisotropy Analysis of Single-Ion Magnets Using an Effective Electrostatic Model. Inorganic Chemistry. 53, pp. 11323 - 11327. 2014. ISSN 0020-1669
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Source of citations: WOS **Citations:** 22

30 J.J. Baldovi; S. Cardona-Serra; J.M. Clemente-Juan; E. Coronado; A. Gaita-Arino; H. Prima-Garcia. Coherent manipulation of spin qubits based on polyoxometalates: the case of the single ion magnet [GdW30P5O110](14-). Chemical Communications. 49 - 79, pp. 8922 - 8924. Royal Society of Chemistry, 2013.
Type of production: Scientific paper
Source of citations: WOS **Citations:** 28

31 J. J. Baldoví; S. Cardona-Serra; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño. Modeling the properties of Uranium-based Single Ion Magnets. Chemical Science. 4, pp. 938 - 946. RSC, 2013. Available on-line at: <DOI:10.1039/C2SC21490C>.

Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Impact source: Journal Webpage **Category:** CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 7,525 **Journal in the top 25%:** Yes
Source of citations: WOS **Citations:** 48

32 S. Cardona-Serra; J.M. Clemente-Juan; A. Gaita-Arino; N. Suaud; O. Svoboda; E. Coronado. Modelling electric field control of the spin state in the mixed-valence polyoxometalate [GeV14O40](8-). Chemical Communications. 49 - 83, pp. 9621 - 9623. Royal Society of Chemistry, 2013.

Type of production: Scientific paper
Source of citations: WOS **Citations:** 10

33 J. J. Baldoví; S. Cardona-Serra; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño. SIMPRE: A Software Package to Calculate Crystal Field Parameters, Energy Levels and Magnetic Properties on Mononuclear Lanthanoid Complexes Based on Charge Distributions. Journal of Computational Chemistry. Wiley, 2013. Available on-line at: <JCC-23341>.

Type of production: Scientific paper **Format:** Journal
Impact source: Journal Webpage
Impact index in year of publication: 4,583
Source of citations: WOS **Citations:** 40

34 J. J. Baldoví; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño. Two pyrazolylborate dysprosium(III) and neodymium(III) single ion magnets modeled by a Radial Effective Charge approach. Polyhedron. Elsevier, 2013. Available on-line at: <DOI:10.1016/j.poly.2013.01.034>.

Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
Impact source: Journal Webpage **Category:** CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 2,057
Source of citations: WOS **Citations:** 14
Relevant publication: No

35 B. Tsukerblat; A. Palii; J.M. Clemente-Juan; A. Gaita-Ariño; E. Coronado. A symmetry adapted approach to the dynamic jahn-teller problem: application to mixed-valence polyoxometalate clusters with keggin structure. International Journal of Quantum Chemistry. 112, pp. 2957 - 2964. (United States of America): 2012. ISSN 0020-7608

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 3

36 C. Bosch Serrano; J. M. Clemente Juan; E. Coronado; A. Gaita Ariño; A. Palii; Boris Tsukerblat. Electric field control of the spin state in mixed-valence magnetic molecules. Chemphyschem. 13, pp. 2662 - 2665. (Germany): 2012. ISSN 1439-4235

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 12

37 J. J. Baldoví; J. J. Borrás-Almenar; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño. Modeling the properties of lanthanide Single-ion magnets using an effective point-charge approach. Dalton Transactions. 41, pp. 13705 - 13710. (United Kingdom): 2012. ISSN 1477-9226

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 65

38 C. Bosch-Serrano; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; A. Palii; B. Tsukerblat. Molecular analog of multiferroics: Electric and magnetic field effects in many-electron mixed-valence dimers. Physical Review B. 86, pp. 024432. (United States of America): 2012. ISSN 1098-0121

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 13

39 Ghosh, S.; Datta, S.; Friend, L.; Cardona-Serra, S.; Gaita-Ariño, A.; Coronado, E.; Hill. S.Multi-frequency EPR studies of a mononuclear holmium single-molecule magnet based on the polyoxometalate [HoIII(W5O18)2]9−. Dalton Transactions. 41, pp. 13697 - 13704. (United Kingdom): 2012. ISSN 1477-9226

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 31

40 J. J. Baldoví; S. Cardona-Serra; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; A. Palii. Rational Design of Single-Ion Magnets and Spin Qubits Based on Mononuclear Lanthanoid Complexes. Inorganic Chemistry. (United States of America): 2012. ISSN 0020-1669

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 107

41 M. J. Martínez-Pérez; S. Cardona-Serra; C. Schlegel; F. Moro; P. J. Alonso; H. Prima-García; J. M. Clemente-Juan; M. Evangelisti; A. Gaita-Ariño; J. Sesé; J. van Slageren; E. Coronado; F. Luis. Gd-Based single-ion magnets with tunable magnetic anisotropy: molecular design of spin qubits. Physical Review Letters. 108, (United States of America): 2012. Available on-line at: <http://prl.aps.org/abstract/PRL/v108/i24/e247213>. ISSN 0031-9007

Type of production: Scientific paper **Format:** Journal
Impact source: ISI **Category:** PHYSICS, MULTIDISCIPLINARY
Impact index in year of publication: 7,37 **Journal in the top 25%:** Yes
Source of citations: WOS **Citations:** 70
Relevant publication: No

42 S. Cardona-Serra; J. M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; A. Camon; M. Evangelisti; F. Luis; M. J. Martínez-Perez; J. Sese. Lanthanoid Single-Ion Magnets Based on Polyoxometalates with a 5fold Symmetry: The Series [LnP5W30O110]12- (Ln3+ = Tb, Dy, Ho, Er, Tm, and Yb). Journal of the American Chemical Society. 134, pp. 14982 - 14990. (United States of America): 2012. ISSN 0002-7863

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 120
Relevant publication: No

43 A. Palii; B. Tsukerblat; J.M. Clemente-Juan; A. Gaita-Ariño; E. Coronado. Manipulation of the spin in single molecule magnets via Landau-Zener transitions. Physical Review B. 84, pp. 184426. (United States of America): 2011. ISSN 1098-0121

Type of production: Scientific paper **Format:** Journal
Source of citations: WOS **Citations:** 4

44 A. Gaita Ariño; M. Schechter. Identification of strong and weak interacting two level systems in KBr:CN. Physical Review Letters. 107, pp. 105504 - 105509. (United States of America): 2011. Available on-line at: <http://arxiv.org/abs/1012.1852>. ISSN 0031-9007

Type of production: Scientific paper
Format: Journal
Impact source: ISI
Category: PHYSICS, MULTIDISCIPLINARY
Impact index in year of publication: 7,37
Journal in the top 25%: Yes
Relevant publication: No

45 J. M. Clemente-Juan; E. Coronado; A. Forment-Aliaga; A. Gaita-Ariño; C. Giménez-Saiz; F. M. Romero; W. Wernsdorfer; R. Biagi; V. Corradini. Electronic and Magnetic Study of Polycationic Mn12 Single-Molecule Magnets witha Ground Spin State S = 11. Inorganic Chemistry. 49, pp. 386 - 396. (United States of America): 2010. ISSN 0020-1669

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, INORGANIC & NUCLEAR
Impact index in year of publication: 4,325
Journal in the top 25%: Yes
Position of publication: 5
Source of citations: WOS
Citations: 5
Relevant results: Cover of the journal.

46 J. Lehmann; A. Gaita-Ariño; E. Coronado; D. Loss. Quantum computing with molecular spin systems. Journal of Materials Chemistry. 19, pp. 1672 - 1677. (United Kingdom): 2009. ISSN 0959-9428

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, PHYSICAL
Impact index in year of publication: 4,795
Journal in the top 25%: Yes
Source of citations: WOS
Citations: 85

47 P. C. E. Stamp; A. Gaita Ariño. Spin-based quantum computers made by chemistry: hows and whys. Journal of Materials Chemistry. 19, pp. 1718 - 1730. (United Kingdom): 2009. ISSN 0959-9428

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: MATERIALS SCIENCE, MULTIDISCIPLINARY
Impact index in year of publication: 4,795
Journal in the top 25%: Yes
Position of publication: 18
Source of citations: WOS
Citations: 149

48 C.J. Calzado; J.M.Clemente-Juan; E. Coronado E; A. Gaita-Arino; N- Suaud. Role of the electron transfer and magnetic exchange interactions in the magnetic properties of mixed-valence polyoxovanadate complexes. Inorganic Chemistry. 47, pp. 5889 - 5901. (United States of America): 2008. ISSN 0020-1669

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, INORGANIC & NUCLEAR
Impact index in year of publication: 4,147
Journal in the top 25%: Yes
Source of citations: WOS
Citations: 42

49 J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; N. Suaud. Mixed-Valence Polyoxometalates: Spin-Coupling and Electrón Distribution in the Decawolframate Anion Reduced by Two Electrons. Journal of Physical Chemistry A. 111, pp. 9969 - 9977. (United States of America): 2007. ISSN 1089-5639

Type of production: Scientific paper
Format: Journal

Impact source: SCI
Category: PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Impact index in year of publication: 2,918
Journal in the top 25%: Yes
Position of publication: 6
Source of citations: WOS
Citations: 13

50 ML Tong; CG Hong; LL Zheng; MX Peng; A. Gaita-Ariño; JM Clemente Juan. New reactivity of 4-amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole: Synthesis and structure of a mononuclear species, a dinuclear species, and a novel tetranuclear nickel(II) rectangle box, and magnetic properties of the dinuclear and tetranuclear complexes. European Journal of Inorganic Chemistry. 23, pp. 3710 - 3717. 2007.
Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, INORGANIC & NUCLEAR
Impact index in year of publication: 2,597
Position of publication: 11
Source of citations: WOS
Citations: 39

51 J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; C. Giménez-Saiz; H.-U. Güdel; A. Sieber; R. Birchner; H. Mutka. Magnetic Polyoxometalates: Anisotropic Exchange Interactions in the CoII3 Moiety of [(NaOH2)Co3(H2O)(P2W15O56)2]17-. Inorganic Chemistry. 44, pp. 3389 - 3395. (United States of America): 2005. ISSN 0020-1669
Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, INORGANIC & NUCLEAR
Impact index in year of publication: 3,851
Journal in the top 25%: Yes
Position of publication: 6
Source of citations: WOS
Citations: 66
Relevant results: Cover of the journal.

52 N. Suaud; A. Gaita-Ariño; J.M. Clemente-Juan; E. Coronado. Electron Delocalization and Electrostatic Repulsion at the Origin of the Strong Spin Coupling in Mixed-Valence Keggin Polyoxometalates: Ab Initio Calculations of the One- and Two-Electron Processes. Chemistry-A European Journal. 10, pp. 4041 - 4053. (Germany): 2004. ISSN 0947-6539
Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 4,517
Journal in the top 25%: Yes
Position of publication: 10
Source of citations: WOS
Citations: 32

53 E. Coronado; A. Forment-Aliaga; A. Gaita-Ariño; C. Giménez-Saiz; F.M. Romero; W. Wernsdorfer. Polycationic Mn12 Single-Molecule Magnets as Electron Reservoirs with S>10 Ground States.Angewandte Chemie-International Edition. 43, pp. 6152 - 6156. (Germany): 2004. ISSN 1433-7851
Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 9,161
Journal in the top 25%: Yes
Position of publication: 4
Source of citations: WOS
Citations: 60
Relevant publication: No

54 N. Suaud; A. Gaita-Arino; J.M. Clemente-Juan; J. Sanchez-Marin; E.Coronado. Ab initio calculations of the transfer parameters and coulombic repulsion and estimation of their effects on the electron delocalization and magnetic coupling in mixed-valence Keggin polyoxotungstates. Polyhedron. 22, pp. 2331 - 2337. (United Kingdom): 2003. ISSN 0277-5387

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, INORGANIC & NUCLEAR
Impact index in year of publication: 1,584
Journal in the top 25%: No
Position of publication: 18
Source of citations: SCOPUS
Citations: 8

55 A. Forment-Aliaga; E. Coronado; M. Feliz; A. Gaita-Ariño; R. Llusar; F. M. Romero. Cationic Mn12 Single-Molecule Magnets and their polyoxometalate Hybrid Salts.Inorganic Chemistry. 42, pp. 8019 - 8027. (United States of America): 2003. ISSN 0020-1669

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, INORGANIC & NUCLEAR
Impact index in year of publication: 3,389
Journal in the top 25%: Yes
Position of publication: 6
Source of citations: WOS
Citations: 39

56 J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; C. Giménez-Saiz; G. Chaboussant; H.-U. Güdel; R. Burriel; H. Mutka. Magnetism in Polyoxometalates: Anisotropic Exchange Interactions in the Trimeric CoII Moiety [Co3W(D2O)2(ZnW9O34)2]12-. A Magnetic and Inelastic Neutron Scattering Study. Chemistry-A European Journal. 8, pp. 5701 - 5708. (Germany): 2002. ISSN 0947-6539

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 4,238
Journal in the top 25%: Yes
Position of publication: 9
Source of citations: WOS
Citations: 38

57 N. Suaud; A. Gaita-Ariño; J.M. Clemente-Juan; J. Sánchez-Marín; E. Coronado. Electron delocalization in mixed-valence Keggin polyoxometalates. Ab initio calculation of the local effective transfer integrals and its consequences on the spin coupling. Journal of the American Chemical Society. 124, pp. 15134 - 15140. (United States of America): 2002. ISSN 0002-7863

Type of production: Scientific paper
Format: Journal
Impact source: SCI
Category: CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 6,201
Journal in the top 25%: Yes
Position of publication: 5
Source of citations: WOS
Citations: 58
Relevant publication: No

58 J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño. Magnetic Polyoxometalates. Polyoxometalate Molecular Science. 98, pp. 273 - 296. (Holland): Kluwer Academic/Plenum Publishers, 2003. ISBN 978-1-4020-1242-6

Type of production: Book chapter
Format: Book

59 J. M. Clemente-Juan; M. Clemente-León; E. Coronado; A. Forment; A. Gaita; C.J. Gómez-García; E. Martínez-Ferrero. Polyoxometalates: From magnetic models to multifunctional materials. Polyoxometalate chemistry for nano-composite design. pp. 157 - 168. (United States of America): Kluwer Academic/Plenum Publishers, 2002. ISBN 0-306-47359-3

Type of production: Book chapter **Format:** Book

60 J.J. Borrás-Almenar; E. Coronado; A. Gaita-Ariño. "Clusters magnéticos de alta nuclearidad. Modelos en clusters de valencia mixta.". Los materiales moleculares en España en el umbral del siglo XXI. pp. 725 - 727. (Spain): Ediciones de la Universidad Autónoma de Madrid, 2001. ISBN 84-7477-787-9
Legal deposit: M-27297-2001
Type of production: Book chapter **Format:** Book

Works submitted to national or international conferences

1 **Title of the work:** Recent results on magnetic polyoxometalates as spin qubits
Name of the conference: Frontiers in Metal Oxide Cluster Science V
Corresponding author: Yes
City of event: Changchun, China
Date of event: 20/08/2017
End date: 24/08/2017
Organising entity: Northeast Normal University, Jinlin University
City organizing entity: Changchun, China

2 **Title of the work:** Coherence and Organisation in Lanthanoid Spin Qubits
Name of the conference: ICMM 2016 (15th International Conference on Molecule-Based Magnets)
Date of event: 2016
Type of contribution: Scientific book or monograph
Alejandro Gaita-Ariño.

3 **Title of the work:** Short-term highly coherent quantum storage in [GdW30P5O110]12-
Name of the conference: ECMolS
Date of event: 2016
A. Gaita-Ariño.

4 **Title of the work:** A molecular approach to spin qubits: decoherence and organisation in Single-Ion-Magnets
Name of the conference: Workshop 'Información Cuántica en España-1'
Date of event: 2014
A. Gaita-Ariño; J. J. Baldoví; L. Escalera-Moreno; H. Prima-García; G. Mínguez-Espallargas; J. M. Clemente-Juan; E. Coronado.

5 **Title of the work:** Characterization and coherent control of the spin state in single-ion magnets
Name of the conference: 14th International Conference on Molecule-based Magnets
Date of event: 2014
A. Gaita-Ariño; J. J. Baldoví; L. Escalera-Moreno; H. Prima-García; G. Mínguez-Espallargas; N. Suaud; K. van Hoogdalem; J. M. Clemente-Juan; D. Loss; E. Coronado.

6 **Title of the work:** Quantum error correction in a magnetic molecule
Name of the conference: 10th International Workshop on Magnetism and Superconductivity at the Nanoscale COMA-RUGA 2014
Date of event: 2014
A. Gaita-Ariño.

7 **Title of the work:** Magnetic polyoxometalates as hardware for studies in quantum computing
Name of the conference: 1st European Conference on Polyoxometalate Chemistry for Molecular Nanoscience
Geographical area: European Union
Type of participation: Participatory - oral communication
City of event: Tenerife, Spain
Date of event: 16/05/2013
End date: 19/05/2013
Alejandro Gaita Ariño; José J. Baldoví; Salvador Cardona Serra; Juan M. Clemente Juan; Eugenio Coronado; Fernando Luis; Helena Prima García.

8 **Title of the work:** Theoretical calculations of spin dynamics and quantum effects in rare earth SMMs
Name of the conference: APS March Meeting 2013
Geographical area: Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Baltimore, United States of America
Date of event: 2013
Organising entity: American Physical Society
Alejandro Gaita Ariño.

9 **Title of the work:** Electric field control of the spin in mixed-valence magnetic molecules
Name of the conference: 40 International Conference on Coordination Chemistry (ICCC40)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 09/09/2012
End date: 13/09/2012
C. Bosch Serrano; J. M. Clemente Juan; A. Gaita Ariño; A. Palii; B. Tsukerblat; E. Coronado.

10 **Title of the work:** Lanthanoid complexes for quantum error correction
Name of the conference: 40 International Conference on Coordination Chemistry (ICCC40)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 09/09/2012
End date: 13/09/2012
A. Gaita Ariño; J.J. Baldoví; S. Cardona Serra; J. M. Clemente Juan; E. Coronado; G. Mínguez Espallargas.

11 **Title of the work:** Mixed-valence polyoxometalates: use of symmetry in the dynamic vibronic problem
Name of the conference: 40 International Conference on Coordination Chemistry (ICCC40)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 09/09/2012
End date: 13/09/2012
J. M. Clemente Juan; A. Gaita Ariño; E. Coronado; A. Palii; B. Tsukerblat.

12 **Title of the work:** Rational Design of Single Ion Magnets and Spin Qubits Based on Mononuclear Lanthanoid Complexes
Name of the conference: 40 International Conference on Coordination Chemistry (ICCC40)
Geographical area: Non EU International

Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 09/09/2012
End date: 13/09/2012
J. J. Baldoví; S. Cardona Serra; J. M. Clemente Juan; E. Coronado; A. Gaita Ariño; A. Palii.

13 **Title of the work:** SMMs Behaviour in Magnetic Polyoxometalates
Name of the conference: 40 International Conference on Coordination Chemistry (ICCC40)
Geographical area: Non EU International
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 09/09/2012
End date: 13/09/2012
S. Cardona Serra; J. M. Clemente Juan; E. Coronado; A. Gaita Ariño.

14 **Title of the work:** Polyoxometalates as spin qubits
Name of the conference: Frontiers in Metal-Oxide Cluster Science 2012
Type of event: Conference
Type of participation: Participatory - invited/keynote talk
City of event: Lanzarote, Spain
Date of event: 2012
Alejandro Gaita Ariño.

15 **Title of the work:** Shor's quantum error correction using a single molecule
Name of the conference: Workshop 'Información Cuántica en España'
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Madrid, Spain
Date of event: 2012
Alejandro Gaita Ariño.

16 **Title of the work:** Identifying Two-Level-Systems: from K:Br:CN to Ar:N2
Name of the conference: Israel Physical Society Conference 2011
Type of event: Conference
Type of participation: Participatory - invited/keynote talk
City of event: Haifa, Israel
Date of event: 2011
Alejandro Gaita-Ariño; Vicente González-Albuixec; Moshe Schechter.

17 **Title of the work:** Magnetic polyoxometalates in molecular electronics
Name of the conference: 2010 International Chemical Congress of Pacific Basin Societies
Type of event: Conference
Type of participation: Participatory - invited/keynote talk
City of event: Honolulu, United States of America
Date of event: 2010
J.M. Clemente-Juan; S. Cardona-Serra; E. Coronado; A. Gaita-Ariño; N. Suaud; J.J. Palacios.

18 **Title of the work:** Polyoxometalates as spin qubits
Name of the conference: March Meeting of the American Physical Society
Type of event: Conference
Type of participation: Participatory - oral communication

City of event: New Orleans, United States of America
Date of event: 2008
Alejandro Gaita-Arino; M. A. AlDamen; J.-M. Clemente-Juan; E. Coronado; J. Lehmann; D. Loss; P. Stamp.

19 **Title of the work:** Spin qubits with electrically gated polyoxometalate molecules
Name of the conference: European Materials Research Society 2007 Spring Meeting
Type of event: Conference
Type of participation: Participatory - invited/keynote talk
City of event: Strassbourg, France
Date of event: 2007
J. Lehmann; A. Gaita-Ariño; E. Coronado; D. Loss.

20 **Title of the work:** Magnetic Properties of High-Nuclearity Mixed-Valence Clusters
Name of the conference: European Conference on Molecular Magnetism, ECMM
Type of participation: Participatory - oral communication
City of event: Tomar, Portugal
Date of event: 10/10/2006
End date: 15/10/2006
M. A. AlDamen; J. M. Clemente Juan; E. Coronado; A. Gaita.

21 **Title of the work:** Evaluation of effective hamiltonians for high nuclearity magnetic clusters
Name of the conference: India-European Thematic Meeting on Computational Materials Science
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Bangalore, India
Date of event: 2006
J.M. Clemente-Juan; A. Gaita-Ariño; M.A. AlDAmen; E. Coronado; N. Suaud.

22 **Title of the work:** Modelling high nuclearity mixed-valence magnetic clusters
Name of the conference: 10th International Conference on Molecule-Based Magnets
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Victoria, B.C., Canada
Date of event: 2006
M.A. AlDAmen; J.M. Clemente-Juan; E. Coronado; A. Gaita-Ariño; C. Calzado; N. Suaud.

23 **Title of the work:** Magnetic Properties of High-Nuclearity Mixed-Valence Clusters
Name of the conference: Internacional Symposium on Nano-structures and Physicochemical Properties of Polyoxometalates, Superclusters and Related Colloid Particles
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Lion, France
Date of event: 2005
Juan M. Clemente-Juan; A. Gaita-Ariño; M.A. AlDamen; E. Coronado; N. Suaud; C. Calzado.

24 **Title of the work:** The origin of the diamagnetism of 2-electron-reduced polyoxometalates: An ab initio + model Hamiltonian calculations approach
Name of the conference: Internacional Symposium on Nano-structures and Physicochemical Properties of Polyoxometalates, Superclusters and Related Colloid Particles
Type of event: Conference
Type of participation: Participatory - oral communication

City of event: Lion, France
Date of event: 2005
N. Suaud; A. Gaita-Ariño; J. M. Clemente-Juan; E. Coronado.

25 **Title of the work:** Magnetic Properties of High-Nuclearity Mixed-Valence Clusters. Theoreticall Approaches.
Name of the conference: IXth International Conference on Molecule-based Magnets (ICMM2004)
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Tsukuba, Japan
Date of event: 2004
A. Gaita-Ariño; N. Suaud; J.M. Clemente-Juan; E. Coronado; C. Calzado.

26 **Title of the work:** Magnetism in high-nuclearity mixed-valencia clusters
Name of the conference: International Conference on Magnetism, ICM2003
Type of participation: 'Participatory - poster
City of event: Roma, Italy
Date of event: 04/10/2003
End date: 08/10/2003
A. Gaita Ariño; N. Suaud; J. M. Clemente Juan; E. Coronado; C. Calzado.

27 **Title of the work:** Anisotropic exchange in the trimeric cluster [Co3W(D2O)2(ZnW9O34)2]12-. A magnetic and inelastic neutron scattering study
Name of the conference: VIIIth International conference on molecule based magnets. ICMM 2002
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 05/10/2002
End date: 10/10/2002
J.M. Clemente Juan; A. Gaita Ariño; E. Coronado; G. Chaboussant; H. U. Güdel; H. Mutka.

28 **Title of the work:** Electron delocalization in mixed-valence a-PW12O405- Keggin polyoxometalate reduced by two electrons
Name of the conference: VIIIth International conference on molecule based magnets. ICMM 2002
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 05/10/2002
End date: 10/10/2002
A. Gaita Ariño; N. Suaud; J.M. Clemente Juan; J. Sánchez Marín; E. Coronado.

29 **Title of the work:** Electron Delocalization in □-PW12O40 Mixed-Valence Keggin Polyoxometalate Reduced by Two Electrons
Name of the conference: Journée NanoMat
Type of participation: Participatory - oral communication
City of event: Toulouse, France
Date of event: 10/2002
N. Suaud; A. Gaita Arino; J.M. Clemente Juan; J. Marin Sánchez; E. Coronado.

30 **Title of the work:** Ab initio calculations on electron transfer phenomena in mixed-valence polyoxometalates
Name of the conference: Universidad Autónoma de Madrid - IX International Summer School Nicolás Cabrera: 'Molecular Electronics'
Type of event: Conference
Type of participation: 'Participatory - poster

City of event: Miraflores de la Sierra, Spain
Date of event: 2002
Juan-Modesto Clemente-Juan; Eugenio Coronado; Alejandro Gaita-Ariño; Nicolas Suaud.

31 **Title of the work:** Electron Delocalization in Mixed-Valence α-PW12O40 Keggin Polyoxometalate Reduced by Two Electrons
Name of the conference: Universitat de Valencia - VIIIth International Conference on Molecule-Based Magnets
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Valencia, Spain
Date of event: 2002
Juan-Modesto Clemente-Juan; Eugenio Coronado; Alejandro Gaita-Ariño; Nicolas Suaud.

32 **Title of the work:** One and two electron processes and magnetic properties of mized-valence Keggin polyoxometalates. An ab initio evaluation of the main interactions between delocalized electrons
Name of the conference: X INTERNATIONAL SUMMER SCHOOL “NICOLAS CABRERA”
Type of participation: Participatory - oral communication
City of event: Miraflores de la Sierra, Community of Madrid, Spain
Date of event: 2002
J. M. Clemente Juan; E. Coronado; A. Gaita Ariño; N. Suaud.

33 **Title of the work:** Electron Delocalization, Vibronic Coupling and Magnetic Interactions in Molecular Mixed Valence Magnetic Systems
Name of the conference: European Science Foundation 'Molecular Magnets' Mid-Term conference
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Davos, Switzerland
Date of event: 2001
Alejandro Gaita-Ariño; Boris Tsukerblat; Eugenio Coronado."Libro de resúmenes".

34 **Title of the work:** Espectroscopía con neutrones: síntesis, caracterización y modelización de polioxometalatos magnéticos
Name of the conference: Universidad de Valencia - V Escuela Nacional de Materiales Moleculares
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Peñíscola, Spain
Date of event: 2001
Eugenio Coronado; Juan-Modesto Clemente-Juan; Alejandro Gaita-Ariño; Hans-Ulrich Güdel. "Libro de resúmenes".

35 **Title of the work:** Neutron spectroscopy: synthesis, characterization and modelization of magnetic polyoxometalates
Name of the conference: TRM Network 'Molecules as Nanomagnets' Mid Term Review Meeting
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Dourdan, France
Date of event: 2001
Juan-Modesto Clemente-Juan; Eugenio Coronado; Alejandro Gaita-Ariño; Hans-Ulrich Güdel.

36 **Title of the work:** Espectroscopia con neutrones: Síntesis, caracterización y modelización de polioxometalatos magnéticos
Name of the conference: Oxides. Physico-chemical properties
Type of participation: Participatory - oral communication
City of event: Ekaterinburg, Russia
Date of event: 22/02/2000
End date: 25/02/2000
E. Coronado; J. M. Clemente Juan; A. Gaita Ariño; H. U. Güdel.

37 **Title of the work:** Electronic Delocalization and Vibronic Coupling in Mixed-Valence Spin Clusters
Name of the conference: European Science Foundation Seminar 'Molecular Magnets II'
Type of event: Conference
Type of participation: Participatory - oral communication
City of event: Lübeck, Germany
Date of event: 2000
Eugenio Coronado; Alejandro Gaita-Ariño; Boris Tsukerblat.

38 **Title of the work:** Mixed-Valence Clusters V18O42n-. Theoretical Models.
Name of the conference: Theoretical Aspects of Molecular Magnetism
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Knokke-Zoute, Belgium
Date of event: 1999
Juan-José Borrás-Almenar; Juan-Modesto Clemente-Juan; Eugenio Coronado; Alejandro Gaita-Ariño.

39 **Title of the work:** High Nuclearity Magnetic Clusters. Models in Spin Clusters and in Mixed Valence Clusters
Name of the conference: Molecular Clusters: Magnetism and Quantum Size Effects. ESF Workshop
Geographical area: European Union
Type of participation: 'Participatory - poster
City of event: Florencia, Italy
Date of event: 28/11/1998
End date: 01/12/1998
J. J. Borrás Almenar; J. M. Clemente Juan; E. Coronado; A. Gaita; B. S. Tsukerblat.

Other achievements

Stays in public or private R&D centres

1 **Entity:** University of British Columbia **Type of entity:** University
Faculty, institute or centre: Pacific Institute of Theoretical Physics / Department of Physics and Astronomy
City of entity: Vancouver, Canada
Start-End date: 01/09/2007 - 31/08/2010 **Duration:** 3 years
Goals of the stay: Post-doctoral
Provable tasks: Development of a scheme in the framework 'molecular approaches to quantum computing and decoherence'

2 **Entity:** Université Paul Sabatier **Type of entity:** University
Faculty, institute or centre: IRSAMC
City of entity: Toulouse, Midi-Pyrénées, France
Start-End date: 01/10/2005 - 31/03/2006 **Duration:** 6 months
Goals of the stay: Otros (especificar) - Proyecto europeo MagManet
Provable tasks: Ab-initio spectroscopic calculations on mixed-valence polyoxometalates. Electron transfer, coulombic repulsion magnetic exchange.

3 **Entity:** Université Paul Sabatier **Type of entity:** University
Faculty, institute or centre: IRSAMC
City of entity: Toulouse, Midi-Pyrénées, France
Start-End date: 2005 - 2005 **Duration:** 1 month
Goals of the stay: Otros (especificar) - Proyecto europeo MagManet
Provable tasks: Ab-initio spectroscopic calculations on mixed-valence polyoxometalates. Electron transfer, coulombic repulsion magnetic exchange.

4 **Entity:** Institut für Physik
City of entity: Basel, Switzerland
Start date: 2006 **Duration:** 1 month
Goals of the stay: Otros (especificar) - Proyecto europeo MagManet
Provable tasks: Development of a scheme in the framework 'molecular approaches to quantum computing'

5 **Entity:** Institut für Physik
City of entity: Basel, Switzerland
Start date: 2006 **Duration:** 2 months
Goals of the stay: Otros (especificar) - Proyecto europeo MagManet
Provable tasks: Development of a scheme in the framework 'molecular approaches to quantum computing'

Obtained grants and scholarships

1 **Name of the grant:** BECA Organismo: Universitat de València - Estudi General Finalidad: Beca de colaboración. Centro: Instituto de Ciencia Molecular (UVEG).
Conferral date: 01/01/2004 **Duration:** 6 months

2 **Name of the grant:** BECA Organismo: Generalitat Valenciana Finalidad: Tesis Doctoral. Centro: Departamento de Química Inorgánica e Instituto de Ciencia Molecular (UVEG).
Conferral date: 01/01/2000 **Duration:** 4 years

3 **Name of the grant:** BECA: -Organismo: Ministerio de Educación y Ciencia. -Finalidad: Beca de colaboración. -Centro: Departamento de Química Inorgánica (UVEG).
Conferral date: 01/09/1999 **Duration:** 1 year

Summary of other achievements

1 **Description of the achievement:** Referee for Elsevier
Conferral date: 2013

2 **Description of the achievement:** Full-page outreach paper in 'Diagonal' journal (circulation: 20.000); Alejandro Gaita Ariño: "Charlatanes que llaman cuántica a lo que no lo es", nº 171, p. 24 (2012)
Conferral date: 29/03/2012

3 **Description of the achievement:** Referee for the American Chemical Society
Conferral date: 2012

4 **Description of the achievement:** Teacher of intensive lectures (3h) on 'Advanced Computational Techniques' in the European Master in Theoretical Chemistry and Computational Modelling. With the support of the Erasmus Mundus programme of the European Union.
Accrediting entity: Universitat de València
Conferral date: 14/09/2011

5 **Description of the achievement:** Research outreach: Invited speaker at the "Jornada sobre oportunidades para investigadores en el 7º Programa Marco de I+D en la UE"
Accrediting entity: Universitat de València **Type of entity:** University
Conferral date: 2011

6 **Description of the achievement:** Attendance to Scientific Meetings: First Conference on Functional Nanostructures -Place: Karlsruhe (Germany) -Organizer: Centrum für Funktionelle Nanostrukturen - Universität Karlsruhe
Conferral date: 29/09/2003

7 **Description of the achievement:** Attendance to Scientific Meetings: Advanced Physics and Chemistry of Materials -Place: Grenoble (Francia) -Organizer: Université Joseph Fourier
Conferral date: 03/09/2001

8 **Description of the achievement:** Attendance to Scientific Meetings: Teoría Cuántica de la Información -Place: Santiago de Compostela (Spain) -Organizer: Universidad de Santiago de Compostela
Conferral date: 03/09/2001

9 **Description of the achievement:** Attendance to Scientific Meetings: Summerschool on computational quantum chemistry -Place: Milán (Italia) -Organizer: CILEA
Conferral date: 24/07/2000

10 **Description of the achievement:** Attendance to Scientific Meetings: La química a la frontera molecular: noves tecnlogies i modelització -Place: Gandía (España) -Organizer: Universitat de València
Conferral date: 17/07/2000

11 **Description of the achievement:** Attendance to Scientific Meetings: IV Escuela Nacional de Materiales Moleculares -Place: San Lorenzo del Escorial (Madrid) -Organizer: Universidad Autónoma de Madrid-Universidad Complutense de Madrid.
Conferral date: 06/06/1999

12 **Description of the achievement:** Cosupervisor for (ongoing) PhD thesis of José Jaime Baldoví Jachán

13 **Description of the achievement:** Experience with large scientific equipment and facilities: (1) Time-of-Flight Inelastic Neutron Scattering IN6 at the Institut Max von Laue - Paul Langevin (2) Magnetometry with SQUID (3) EPR and pulsed EPR, X band (4) FT-IR spectrometry

14 **Description of the achievement:** Experience with programs and operating systems: (A) User level (1) MOLCAS, CASDI, Boys, NATU (software packages for ab initio spectroscopic calculations) (2) gnuplot, IgorPro, PyX (scientific graphs) (3) awk (data manipulation language) (4) bash (shell script interpreter) (5) unix/GNU toolset (6) fortran77 (scientific programming) (7) Windows XP, Mac OS X, Irix, AIX (OS) (B) Advanced user: (1) magpack, SIMPRE (software packages for the calculation of magnetic properties) (2) Vim (advanced text editor) (3) LaTeX (3) CrystalMaker (crystallography program) (4) Mediawiki, SPIP (C) Administrator level: GNU/Linux (OS)

15 **Description of the achievement:** Teaching experience: - 16 hours, 4th year subject 'Química Inorgánica Avanzada' - 20 hours, 1st year subject 'Operaciones Básicas de Laboratorio'