



Jon Mattin Matxain Beraza

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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.

Mi andadura en mundo de la investigación comenzó en 1996, siendo estudiante Erasmus en la Universidad de Utrecht, Holanda. Allí, me especialicé en Química Teórica y Computacional, obteniendo mi primera publicación científica. Una vez obtenido la titulación de Licenciado, comencé mi tesis doctoral en el grupo de Química Teórica de la Universidad del País Vasco. Allí, estudié las estructuras y propiedades electrónicas y ópticas de nanoclusters semiconductores, concretamente de los materiales llamados II-VI. Durante este periodo, estuve tres meses en el Cavendish Laboratory, de la Universidad de Cambridge. Finalmente, en 2002 defendí mi tesis doctoral como Tesis Europea, obteniendo el Premio Extraordinario de Doctorado.

Posteriormente, en 2005-2006 realicé una estancia postdoctoral de dos años en el grupo de Biofísica Teórica de la Universidad de Örebro, Suecia. Allí, estudié las propiedades antioxidantes de la vitamina B6, concretamente su capacidad de atrapar especies reactivas de oxígeno. Así mismo, continué con la línea de investigación en el ámbito de las nanopartículas, tanto de materiales semiconductores como de nanopartículas metálicas. centrándome en el tuneado de las propiedades ópticas en función del dopaje de estas estructuras, así como en su ensamblado.

En 2009, me incorporé como Investigador Ramón y Cajal en el Grupo de Química Teórica de la UPV/EHU, donde me centré en el estrés oxidativo causado por las especies reactivas de oxígeno, principalmente en proteínas, así como su prevención por antioxidantes. Para ello, además de los métodos estándar de la química computacional, colaboré con el Prof. Piris en el desarrollo de nuevos métodos basados en la teoría del funcional de orbitales naturales. Además de ello, continué con mi investigación sobre la predicción de nuevas nanopartículas y su ensamblado.

Actualmente, soy Investigador Doctor Permanente en la misma Universidad. Gracias a la experiencia obtenida en procesos radicalarios, he iniciado una línea de investigación en el campo de los materiales poliméricos, sobre todo en el diseño de materiales con propiedades de autoreparado. En resumen, hoy en día estoy centrado en dos áreas de investigación: a) el mundo nano y b) el mundo radicalario.

Durante estos casi 20 años de experiencia, he publicado 81 artículos científicos en revistas internacionales de revisión por pares. He publicado 2 capítulos y 1 libro. He tomado parte en una treintena de proyectos de investigación financiados, liderando tres de ellos. Además, he tomado parte en una cuarentena de congresos científicos, impartiendo una veintena de



conferencias invitadas. Así mismo, he sido invitado a impartir otras 6 conferencias en diversos lugares.

En cuanto a la docencia y formación de nuevos investigadores, tengo seis años de experiencia docente, en la que he tomado parte en diez asignaturas, tanto de Licenciatura como de Grado. Así mismo, he dirigido dos tesis doctoral, así como tres tesis de fin de master, y 7 Trabajos de Fin de Grado. Actualmente codirijo 2 Tesis Doctorales, 2 TFM y 5 TFG. Para finalizar, me gustaría mencionar que además de esta labor investigadora y docente, tomo parte activa en la divulgación social de la ciencia en general, y de la química cuántica en particular. Para ello, además del blog asociado a la docencia, colaboro en diversos medios escritos como radiofónicos. Así mismo, soy colaborador de la Cátedra de Cultura Científica de la Universidad del País Vasco.

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.

Total

Sexenios de investigación: 3

Tesis doctorales dirigidas: 2

Tesis de Master: 3

Trabajos de Fin de Grado: 10

Número de publicaciones indexadas: 85

Revistas: 82

Libros y Capítulos de Libros: 3

Publicaciones en Q1: 60 (74%) Índice h (Web of Science: 25; Scopus: 26)

Citas totales (Web of Science: 1785; Scopus: 1879)

Promedio de citas/año (últimos 5 años): (Web of Science: 161; Scopus: 187)

Artículos con 50 o más citas (i50): (Web of Science: 8; Scopus: 8)

Artículos con 10 o más citas (i10): (Web of Science: 54; Scopus: 10)



Jon Mattin Matxain Beraza

Surname(s): **Matxain Beraza**
Name: **Jon Mattin**
DNI: **44623825F**
ORCID: **0000-0002-6342-0649**
Date of birth: **06/08/1975**
Gender: **Male**
Nationality: **Spain**
Country of birth: **Spain**
Aut. region/reg. of birth: **Foral Community of Navarre**
Contact province: **Biscay**
City of birth: **Iruñea / Pamplona**
Contact address: **San Antonio Kalea**
Rest of contact address: **8, 2. ezkerre**
Postcode: **48901**
Contact country: **Spain**
Contact aut. region/reg.: **Basque Country**
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Personal web page: **<http://kimikakuantikoa.blogspot.com.es/>**

Current professional situation

Employing entity: Universidad del País Vasco

Department: Ciencia y Tecnología de Polímeros, Facultad de Ciencias Químicas

Professional category: Personal Investigador Doctor Permanente

Start date: 14/09/2016

Type of contract: Permanent employment contract

Dedication regime: Full time

Primary (UNESCO code): 230700 - Physical chemistry

Previous positions and activities

	Employing entity	Professional category	Start date
1	Universidad del País Vasco	Personal Investigador Doctor	13/01/2014
2	Universidad del País Vasco	Investigador Ramón y Cajal	01/01/2009
3	Universidad del País Vasco	Personal Investigador Contratado Doctor	03/03/2008
4	Universidad del País Vasco	Personal Investigador Contratado Doctor	01/01/2007
5	Universidad de Örebro	Investigador PostDoctoral	01/01/2005
6	Universidad del País Vasco	Investigador PostDoctoral	12/12/2002



- 1** **Employing entity:** Universidad del País Vasco **Type of entity:** University
Professional category: Personal Investigador Doctor
Start-End date: 13/01/2014 - 13/09/2016 **Duration:** 2 years - 9 months
- 2** **Employing entity:** Universidad del País Vasco **Type of entity:** University
Professional category: Investigador Ramón y Cajal
Start-End date: 01/01/2009 - 31/12/2013 **Duration:** 5 years
- 3** **Employing entity:** Universidad del País Vasco **Type of entity:** University
Professional category: Personal Investigador Contratado Doctor
Start-End date: 03/03/2008 - 31/12/2008 **Duration:** 9 months - 28 days
- 4** **Employing entity:** Universidad del País Vasco **Type of entity:** University
Professional category: Personal Investigador Contratado Doctor
Start-End date: 01/01/2007 - 31/12/2007 **Duration:** 1 year
- 5** **Employing entity:** Universidad de Örebro **Type of entity:** University
Professional category: Investigador PostDoctoral
Start-End date: 01/01/2005 - 31/12/2006 **Duration:** 2 years
- 6** **Employing entity:** Universidad del País Vasco **Type of entity:** University
Professional category: Investigador PostDoctoral
Start-End date: 12/12/2002 - 31/12/2004 **Duration:** 2 years - 17 days



Education

University education

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

University degree: Higher degree

Name of qualification: Licenciado en Ciencias Químicas Especialidad Fundamental

Degree awarding entity: Universidad del País Vasco **Type of entity:** University

Date of qualification: 30/06/1998

Doctorates

Doctorate programme: Materiales poliméricos (matpol)

Degree awarding entity: Universidad del País Vasco **Type of entity:** University

City degree awarding entity: Basque Country, Spain

Date of degree: 04/07/2002

DEA awarding entity: Universidad del País Vasco

Date DEA was awarded: 05/06/2000

European doctorate: Yes

Date of certificate: 09/09/2004

Thesis title: Small Clusters of II-VI Materials

Thesis director: Jesus M. Ugalde Uribe-Etxebarria

Obtained qualification: Excellent Cum Laude

Recognition of quality: Yes

Special doctorate award: Yes

Date of award: 09/09/2004

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
Spanish		C1	C1	C1	C1
Basque		C1	C1	C1	C1
English		C1	C1	C1	C1

Teaching experience

General teaching experience

- 1** **Type of teaching:** Official teaching
Name of the course: Química Física I
Professional category: Investigador Doctor Permanente
Type of programme: Bachelor's degree **Type of teaching:** In person theory
Type of subject: Obligatory
University degree: Grado en Ciencias Químicas
Course given: 2
Start date: 09/2017 **End date:** 07/2018
End date: 07/2018 **Type of hours/ ECTS credits:** Credits
Hours/ECTS credits: 6
Entity: Universidad del País Vasco **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias Químicas
Department: Ciencia y Tecnología de Polímeros
City of entity: Donostia, Basque Country, Spain
Subject language: Spanish
- 2** **Type of teaching:** Official teaching
Name of the course: Química Física II
Professional category: Investigador Doctor Permanente
Type of programme: Bachelor's degree **Type of teaching:** In person theory
Type of subject: Obligatory
University degree: Grado en Ciencias Químicas
Course given: 3
Start date: 09/2017 **End date:** 07/2018
End date: 07/2018 **Type of hours/ ECTS credits:** Credits
Hours/ECTS credits: 9
Entity: Universidad del País Vasco **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias Químicas
Department: Ciencia y Tecnología de Polímeros
City of entity: Donostia, Basque Country, Spain
Subject language: Basque
- 3** **Type of teaching:** Official teaching
Name of the course: Química Física II
Professional category: Investigador Doctor Permanente
Type of programme: Bachelor's degree **Type of teaching:** In person theory
Type of subject: Obligatory
Assessment type: Survey
University degree: Grado en Ciencias Químicas
Course given: 3
Start date: 09/2016 **End date:** 07/2017
End date: 07/2017 **Type of hours/ ECTS credits:** Credits
Hours/ECTS credits: 9
Entity: Universidad del País Vasco **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias Químicas
Department: Ciencia y Tecnología de Polímeros
City of entity: Donostia, Basque Country, Spain



Assessment entity: Encuesta Alumnado

Assessment type: Survey

Mark obtained: 4.8

Subject language: Basque

Top mark possible: 5

4 Type of teaching: Official teaching

Name of the course: Química Física II

Professional category: Investigador Ramón y Cajal / Personal Investigador Contratado Doctor

Type of programme: Bachelor's degree

Type of teaching: In person theory

Type of subject: Obligatory

Assessment type: Survey

University degree: Grado en Ciencias Químicas

Course given: 3

Start date: 09/2015

End date: 07/2016

End date: 07/2016

Type of hours/ ECTS credits: Credits

Hours/ECTS credits: 3,94

Entity: Universidad del País Vasco

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias Químicas

Department: Ciencia y Tecnología de Polímeros

City of entity: Donostia, Basque Country, Spain

Assessment entity: Encuesta Alumnado

Assessment type: Survey

Mark obtained: 4.7

Top mark possible: 5

Subject language: Basque

5 Type of teaching: Official teaching

Name of the course: Química Física II

Professional category: Investigador Ramón y Cajal / Personal Investigador Contratado Doctor

Type of programme: Bachelor's degree

Type of teaching: In person theory

Type of subject: Obligatory

Assessment type: Survey

University degree: Grado en Ciencias Químicas

Course given: 3

Start date: 09/2014

End date: 07/2015

End date: 07/2015

Type of hours/ ECTS credits: Credits

Hours/ECTS credits: 2,89

Entity: Universidad del País Vasco

Type of entity: University

Faculty, institute or centre: Facultad de Ciencias Químicas

Department: Ciencia y Tecnología de Polímeros

City of entity: Donostia, Basque Country, Spain

Assessment entity: Encuesta Alumnado

Assessment type: Survey

Mark obtained: 4.5

Top mark possible: 5

Subject language: Basque

6 Type of teaching: Official teaching

Name of the course: Química Física II

Professional category: Investigador Ramón y Cajal / Personal Investigador Contratado Doctor

Type of programme: Bachelor's degree

Type of teaching: In person theory

Type of subject: Obligatory

Assessment type: Survey



University degree: Grado en Ciencias Químicas

Course given: 3

Start date: 09/2013

End date: 07/2014

Hours/ECTS credits: 7,45

Entity: Universidad del País Vasco

Faculty, institute or centre: Facultad de Ciencias Químicas

Department: Ciencia y Tecnología de Polímeros

City of entity: Donostia, Basque Country, Spain

Assessment entity: Encuesta Alumnado

Assessment type: Survey

Mark obtained: 4.6

Subject language: Basque

End date: 07/2014

Type of hours/ ECTS credits: Credits

Type of entity: University

Top mark possible: 5

7 Type of teaching: Official teaching

Name of the course: Química Física Avanzada

Professional category: Investigador Ramón y Cajal

Type of programme: Bachelor's degree

Type of subject: Core

Assessment type: Survey

University degree: Licenciado en Ciencias Químicas

Course given: 4

Start date: 09/2012

End date: 07/2013

Hours/ECTS credits: 3,7

Entity: Universidad del País Vasco

Faculty, institute or centre: Facultad de Ciencias Químicas

Department: Ciencia y Tecnología de Polímeros

City of entity: Donostia, Basque Country, Spain

Assessment entity: Encuesta Alumnado

Assessment type: Survey

Mark obtained: 4.8

Subject language: Basque

Type of teaching: In person theory

End date: 07/2013

Type of hours/ ECTS credits: Credits

Type of entity: University

Top mark possible: 5

8 Type of teaching: Official teaching

Name of the course: Química Física II

Professional category: Investigador Ramón y Cajal / Personal Investigador Contratado Doctor

Type of programme: Bachelor's degree

Type of subject: Obligatory

Assessment type: Survey

University degree: Grado en Ciencias Químicas

Course given: 3

Start date: 09/2012

End date: 07/2013

Hours/ECTS credits: 5,7

Entity: Universidad del País Vasco

Faculty, institute or centre: Facultad de Ciencias Químicas

Department: Ciencia y Tecnología de Polímeros

City of entity: Donostia, Basque Country, Spain

Assessment entity: Encuesta Alumnado

Assessment type: Survey

Type of teaching: In person theory

End date: 07/2013

Type of hours/ ECTS credits: Credits

Type of entity: University



Mark obtained: 4.6
Subject language: Basque

Top mark possible: 5

9 **Type of teaching:** Official teaching
Name of the course: Experimentación Química Física
Professional category: Investigador Ramón y Cajal
Type of programme: Bachelor's degree
Type of subject: Core
Assessment type: Survey
University degree: Licenciado en Ciencias Químicas
Course given: 4
Start date: 09/2011
End date: 07/2012
Hours/ECTS credits: 2,6
Entity: Universidad del País Vasco
Faculty, institute or centre: Facultad de Ciencias Químicas
Department: Ciencia y Tecnología de Polímeros
City of entity: Donostia, Basque Country, Spain
Assessment entity: Encuesta Alumnado
Assessment type: Survey
Mark obtained: 4.7
Subject language: Basque

Type of teaching: Laboratory work

End date: 07/2012
Type of hours/ ECTS credits: Credits

Type of entity: University

Top mark possible: 5

10 **Type of teaching:** Official teaching
Name of the course: Química Física Avanzada
Professional category: Investigador Ramón y Cajal
Type of programme: Bachelor's degree
Type of subject: Core
Assessment type: Survey
University degree: Licenciado en Ciencias Químicas
Course given: 4
Start date: 09/2011
End date: 07/2012
Hours/ECTS credits: 3,7
Entity: Universidad del País Vasco
Faculty, institute or centre: Facultad de Ciencias Químicas
Department: Ciencia y Tecnología de Polímeros
City of entity: Donostia, Basque Country, Spain
Assessment entity: Encuesta Alumnado
Assessment type: Survey
Mark obtained: 4.7
Subject language: Basque

Type of teaching: In person theory

End date: 07/2012
Type of hours/ ECTS credits: Credits

Type of entity: University

Top mark possible: 5

11 **Type of teaching:** Official teaching
Name of the course: Química Física Avanzada
Professional category: Investigador Ramón y Cajal
Type of programme: Bachelor's degree
Type of subject: Core
Assessment type: Survey
University degree: Licenciado en Ciencias Químicas
Course given: 4

Type of teaching: In person theory

**Start date:** 09/2010**End date:** 07/2011**Hours/ECTS credits:** 3,7**Entity:** Universidad del País Vasco**Faculty, institute or centre:** Facultad de Ciencias Químicas**Department:** Ciencia y Tecnología de Polímeros**City of entity:** Donostia, Basque Country, Spain**Assessment entity:** Encuesta Alumnado**Assessment type:** Survey**Mark obtained:** 4.6**Subject language:** Basque**End date:** 07/2011**Type of hours/ ECTS credits:** Credits**Type of entity:** University**Top mark possible:** 5**12 Type of teaching:** Official teaching**Name of the course:** Experimentación Química Física**Professional category:** Investigador Ramón y Cajal**Type of programme:** Bachelor's degree**Type of subject:** Core**Assessment type:** Survey**University degree:** Licenciado en Ciencias Químicas**Course given:** 4**Start date:** 09/2009**End date:** 07/2011**Hours/ECTS credits:** 6**Entity:** Universidad del País Vasco**Faculty, institute or centre:** Facultad de Ciencias Químicas**Department:** Ciencia y Tecnología de Polímeros**City of entity:** Donostia, Basque Country, Spain**Assessment entity:** Encuesta Alumnado**Assessment type:** Survey**Mark obtained:** 4.9**Subject language:** Basque**Type of teaching:** Laboratory work**End date:** 07/2011**Type of hours/ ECTS credits:** Credits**Type of entity:** University**Top mark possible:** 5**13 Type of teaching:** Official teaching**Name of the course:** Experimentación Química Física**Professional category:** Investigador Ramón y Cajal**Type of programme:** Bachelor's degree**Type of subject:** Core**Assessment type:** Survey**University degree:** Licenciado en Ciencias Químicas**Course given:** 4**Start date:** 09/2009**End date:** 09/2010**Hours/ECTS credits:** 6**Entity:** Universidad del País Vasco**Faculty, institute or centre:** Facultad de Ciencias Químicas**Department:** Ciencia y Tecnología de Polímeros**City of entity:** Donostia, Basque Country, Spain**Assessment entity:** Encuesta Alumnado**Assessment type:** Survey**Mark obtained:** 4.8**Subject language:** Basque**Type of teaching:** Laboratory work**End date:** 09/2010**Type of hours/ ECTS credits:** Credits**Type of entity:** University**Top mark possible:** 5

**14 Type of teaching:** Official teaching**Name of the course:** Química Física Avanzada**Professional category:** Investigador Ramón y Cajal**Type of programme:** Bachelor's degree**Type of subject:** Core**Assessment type:** Survey**University degree:** Licenciado en Ciencias Químicas**Course given:** 4**Start date:** 09/2009**End date:** 09/2010**Hours/ECTS credits:** 3,8**Entity:** Universidad del País Vasco**Faculty, institute or centre:** Facultad de Ciencias Químicas**Department:** Ciencia y Tecnología de Polímeros**City of entity:** Donostia, Basque Country, Spain**Assessment entity:** Encuesta Alumnado**Assessment type:** Survey**Mark obtained:** 4.2**Subject language:** Basque**Type of teaching:** In person theory**End date:** 09/2010**Type of hours/ ECTS credits:** Credits**Type of entity:** University**Top mark possible:** 5**Experience supervising doctoral thesis and/or final year projects****1 Project title:** Konposatu Autokonpongarrietan ematen diren disulfuro loturen azterketa teorikoa**Type of project:** End of course project**Co-director of thesis:** Fernando Ruipérez Cillán**Entity:** Universidad del País Vasco**Student:** Maialen Galdeano Fraile**Obtained qualification:** 9.8**Date of reading:** 19/09/2017**European doctorate:** No**Type of entity:** University**2 Project title:** Estudio Teórico de las Propiedades Ópticas del Azuleno**Type of project:** End of course project**Co-director of thesis:** David Casanova Casas**Entity:** Universidad del País Vasco**Student:** Iker Arrieta**Obtained qualification:** 9.8**Date of reading:** 18/07/2017**European doctorate:** No**Type of entity:** University**3 Project title:** Excitaciones Electrónicas Colectivas en Nanoclusters Metálicos**Type of project:** End of course project**Co-director of thesis:** David Casanova Casas**Entity:** Universidad del País Vasco**Student:** Maria Zubiria Ulac**Obtained qualification:** 9.8**Date of reading:** 18/07/2017**European doctorate:** No**Type of entity:** University

- 4** **Project title:** Protein Oxidation by the Attack of OH Radicals
Type of project: Doctoral thesis
Co-director of thesis: 1
Entity: Universidad del País Vasco **Type of entity:** University
Student: Jon Uranga Barandiaran
Obtained qualification: Sobresaliente Cum Laude
Date of reading: 03/07/2017
European doctorate: Yes
Quality recognition: No
- 5** **Project title:** Molecular Quantum Dynamical study of ultra-fast processes on the first two electronic excited states of azulene
Type of project: Master Thesis
Co-director of thesis: 1
Entity: Universidad del País Vasco **Type of entity:** University
Student: Xabier Telleria Allika
Obtained qualification: 10.0
Date of reading: 22/06/2017
European doctorate: No
- 6** **Project title:** Diseño de nuevos materiales nanoporosos basados en el autoensamblado de nanopartículas semiconductoras
Type of project: End of course project
Co-director of thesis: Jesus Ugalde Uribe-Etxebarria
Entity: Universidad del País Vasco **Type of entity:** University
Student: Juan José Gutiérrez Martín
Obtained qualification: 6.4
Date of reading: 23/03/2017
European doctorate: No
- 7** **Project title:** Excitaciones colectivas en clusters de aluminio y derivados
Type of project: End of course project
Co-director of thesis: Jose Javier Lopez Pestaña
Entity: Universidad del País Vasco **Type of entity:** University
Student: Mikel Irigoien
Obtained qualification: 9.3
Date of reading: 22/09/2016
European doctorate: No
- 8** **Project title:** DISULFURO LOTUREN BIDEZ AUTOKONPONTZEKO GAI DIREN MATERIALEN AZTERKETA TEORIKOA
Type of project: End of course project
Co-director of thesis: Jesus M. Ugalde Uribe-Etxebarria
Entity: Universidad del País Vasco **Type of entity:** University
Student: Ekiñe Gimenez
Obtained qualification: 8.8
Date of reading: 20/09/2016
European doctorate: No



- 9** **Project title:** Diseño de nuevas nanopartículas semiconductoras magnéticas
Type of project: End of course project
Co-director of thesis: Jesus M. Ugalde Uribe-Etxebarria
Entity: Universidad del País Vasco **Type of entity:** University
Student: Iker Ortiz de Luzuriaga
Obtained qualification: 8.1
Date of reading: 19/09/2016
European doctorate: No
- 10** **Project title:** Structure and Electronic Properties of Endohedrally Doped II-VI Hollow Nanoclusters
Type of project: Doctoral thesis
Co-director of thesis: Jesus M. Ugalde Uribe-Etxebarria
Entity: Universidad del País Vasco **Type of entity:** University
Student: Elisa Jimenez Izal
Obtained qualification: Excellent Cum Laude
Date of reading: 05/09/2014
European doctorate: Yes **Date of recognition:** 05/09/2014
- 11** **Project title:** Protein Damage by Oxidative Stress
Type of project: Master Thesis
Entity: Universidad del País Vasco **Type of entity:** University
Student: Jon Uranga Barandiaran
Obtained qualification: Sobresaliente
Date of reading: 30/06/2014
- 12** **Project title:** Diseño de novo de nanomateriales semiconductores basados en los fullerenos de los elementos II-VI
Type of project: Master Thesis
Entity: Universidad del País Vasco **Type of entity:** University
Student: Elisa Jimenez Izal
Obtained qualification: Sobresaliente por unanimidad
Date of reading: 22/10/2010

Scientific and technological experience

Research and development groups/teams

- 1** **Name of the group:** Kimika Teorikoa
Name of principal investigator: Jesus M. Ugalde Uribe-Etxebarria
Type of collaboration: Co-authorship of projects and their development
City of group: Donostia, Basque Country, Spain
Affiliation entity: Universidad del País Vasco **Type of entity:** University
Number of directed thesis: 17
Start date: 01/2007 **Duration:** 8 years - 4 months
- 2** **Name of the group:** Theoretical Biophysics Group
Name of principal investigator: Leif A. Eriksson
Type of collaboration: Co-authorship of projects and their development
City of group: Örebro, Sweden
Affiliation entity: Örebro University **Type of entity:** University
Start date: 01/01/2005 **Duration:** 2 years
- 3** **Name of the group:** Theory of Condensed Matter
Name of principal investigator: Richard Needs
Type of collaboration: Co-authorship of projects and their development
City of group: Cambridge, United Kingdom
Affiliation entity: Cavendish Laboratory, Cambridge University **Type of entity:** University
Start date: 07/2001 **Duration:** 3 months
- 4** **Name of the group:** Kimika Teorikoa
Name of principal investigator: Jesus M. Ugalde Uribe-Etxebarria
Type of collaboration: Co-authorship of projects and their development
City of group: Donostia, Basque Country, Spain
Affiliation entity: Universidad del País Vasco **Type of entity:** University
Start date: 10/1998 **Duration:** 6 years - 2 months
- 5** **Name of the group:** Theoretical Chemistry Group
Name of principal investigator: F. B. van Duijneveldt
Type of collaboration: Co-authorship of publications
City of group: Utrecht, Utrecht, Holland
Affiliation entity: Utrecht University **Type of entity:** University
Start date: 09/1996 **Duration:** 2 years

Scientific or technological activities

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

- 1** **Name of the project:** Ayudas Para La Incorporación Estable De Doctores 2017
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jon M Matxain Beraza
Nº of researchers: 1
Funding entity or bodies: Ministerios de Economía y Competitividad **Type of entity:** Gobierno Estado
City funding entity: Madrid, Spain
Type of participation: Principal investigator
Code according to the funding entity: IEDI-2017-00929
Start-End date: 2018 - 2020 **Duration:** 3 years
Total amount: 100.000 €
- 2** **Name of the project:** NANOCCLUSERS METALICOS, COVALENTES Y VAN DER WAALS: ¿ALGO EN COMUN?
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria
Nº of researchers: 6
Funding entity or bodies: Ministerios de Economía y Competitividad **Type of entity:** Gobierno Estado
City funding entity: Madrid, Spain
Type of participation: Team member
Code according to the funding entity: CTQ2015-67660-P
Start-End date: 2016 - 2018 **Duration:** 3 years
Total amount: 98.000 €
- 3** **Name of the project:** Efectos del aluminio en Sistemas Biológicos: Una aproximación computacional
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jose Javier Lopez Pestaña
Funding entity or bodies: Universidad del País Vasco **Type of entity:** University
City funding entity: Bilbao, Basque Country, Spain

**Type of participation:** Others**Code according to the funding entity:** PES14/35**Start-End date:** 2014 - 2018**Duration:** 3 years**Total amount:** 34.586,39 €

- 4 Name of the project:** Theoretical Chemistry and Computational Modelling
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** European Union
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus Maria Ugalde Uribe-Etxebarria
Nº of researchers: 4
Funding entity or bodies: Comisión Europea **Type of entity:** Union Europea
City funding entity: Madrid, Community of Madrid, Spain
Type of participation: Team member
Code according to the funding entity: 642294-TCCM
Start-End date: 2014 - 2018 **Duration:** 4 years
Total amount: 3.000.000 € **Sub-project amount:** 249.876 €

- 5 Name of the project:** Avances en Química Cuántica
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria
Funding entity or bodies: Departamento de Educación y Universidades. Gobierno Vasco **Type of entity:** Gobierno Vasco
Type of participation: Others
Code according to the funding entity: IT588-13
Start-End date: 2013 - 2018 **Duration:** 6 years
Total amount: 401.598 €
- 6 Name of the project:** Interacción del Al(III) con bioligandos y efectos radicalarios en biomoléculas
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jose Javier Lopez Pestaña
Funding entity or bodies: Ministerios de Economía y Competitividad **Type of entity:** Gobierno Estado
City funding entity: Madrid, Spain
Type of participation: Others
Code according to the funding entity: CTQ2012-38496-C05-04
Start-End date: 2013 - 2015 **Duration:** 3 years
Total amount: 28.000 €



- 7** **Name of the project:** Diseño de nuevos materiales nanoporosos basados en el autoensamblado de nanopartículas semiconductoras
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jon M. Matxain Beraza
Nº of researchers: 9
Funding entity or bodies: Departamento de Industria Gobierno Vasco **Type of entity:** Gobierno Vasco
Type of participation: Co-ordinator
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC13UN001
Start-End date: 01/01/2013 - 30/06/2014 **Duration:** 1 year
Total amount: 7.746,7 €
- 8** **Name of the project:** Bases moleculares de la toxicidad del aluminio: afinidad del aluminio por fosfatos de interés biológico y activación de estrés oxidativo
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jose Javier Lopez Pestaña
Funding entity or bodies: Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC13UN003
Start-End date: 2013 - 2014 **Duration:** 1 year
Total amount: 7.746,7 €
- 9** **Name of the project:** Descripción de interacciones no covalentes por medio del método PNOF5-PT2
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Mario Piris Silvera
Funding entity or bodies: Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC13UN005
Start-End date: 2013 - 2014 **Duration:** 1 year
Total amount: 7.746,7 €

- 10** **Name of the project:** Estrategias computacionales para la optimización de celdas solares de inyección directa
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): David Casanova Casas
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC13UN002
Start-End date: 2013 - 2014 **Duration:** 1 year
Total amount: 7.586,39 €
- 11** **Name of the project:** Las especies reactivas de oxígeno (ROS) y la enfermedad de Alzheimer
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jon M. Matxain Beraza
Nº of researchers: 8
Funding entity or bodies:
Departamento de Industria Gobierno Vasco **Type of entity:** Gobierno Vasco
Type of participation: Co-ordinator
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC12UN006
Start-End date: 01/01/2012 - 31/12/2013 **Duration:** 2 years
Total amount: 25.110,59 €
- 12** **Name of the project:** Bioquímica cuantica: Estrés oxidativo en proteínas causado por especies reactivas de oxígeno y nitrógeno y su prevención por antioxidantes
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jon M. Matxain Beraza
Nº of researchers: 1
Funding entity or bodies:
Ministerio de Ciencia e Innovación. Investigación **Type of entity:** Gobierno
City funding entity: Madrid, Community of Madrid, Spain
Type of participation: Principal investigator
Code according to the funding entity: RyC 2008-03216
Start-End date: 01/01/2009 - 31/12/2013 **Duration:** 5 years
Total amount: 192.480 €

- 13** **Name of the project:** Aplicación de la teoría de orbitales naturales a nanopartículas biológicas
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Mario Piris Silvera
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC12UN005
Start-End date: 2012 - 2013 **Duration:** 2 years
Total amount: 25.110,59 €
- 14** **Name of the project:** Diseño de nuevos nanomateriales semiconductores para su posible aplicación en biología
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC12UN003
Start-End date: 2012 - 2013 **Duration:** 2 years
Total amount: 25.110,59 €
- 15** **Name of the project:** Explosiones Culómbicas inducidas por pulsor laser ultraintenso y ultracorto
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Andreas Heidenreich
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC12UN002
Start-End date: 2012 - 2013 **Duration:** 2 years
Total amount: 25.110,59 €

- 16** **Name of the project:** Interacciones no covalentes como pasos preliminares en reacciones químicas
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Slawomir J Grabowski
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC12UN004
Start-End date: 2012 - 2013 **Duration:** 2 years
Total amount: 25.110,59 €
- 17** **Name of the project:** Aplicación de la teoría de orbitales naturales a sistemas biológicos
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Mario Piris Silvera
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC11UN003
Start-End date: 2011 - 2012 **Duration:** 2 years
Total amount: 25.155,08 €
- 18** **Name of the project:** Avances en Química Cuántica y algunas aplicaciones a problemas seleccionados de nanociencia y biofísica
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria
Funding entity or bodies:
Ministerio de Ciencia e Innovación **Type of entity:** Gobierno Estado
City funding entity: Madrid, Community of Madrid, Spain
Type of participation: Others
Code according to the funding entity: CTQ2011-27374
Start-End date: 2011 - 2012 **Duration:** 1 year
Total amount: 14.520 €

- 19** **Name of the project:** Diseño de nanopartículas magnéticas para su aplicación en nano-aparatos
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: S-PC11UN006
Start-End date: 2011 - 2012 **Duration:** 2 years
Total amount: 25.180,08 €
- 20** **Name of the project:** Avances en Química Cuántica
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria
Funding entity or bodies:
Departamento de Educación y Universidades. Gobierno Vasco
Type of participation: Others
Code according to the funding entity: IT33007
Start-End date: 2007 - 2012 **Duration:** 6 years
Total amount: 588.176,61 €
- 21** **Name of the project:** Nanopartículas semiconductoras en entorno biológico: ¿aplicaciones biomédicas?
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Jose Javier Lopez Pestaña
Funding entity or bodies:
Departamento de Industria. Gobierno Vasco **Type of entity:** Gobierno Vasco
City funding entity: Basque Country, Spain
Type of participation: Others
Name of the programme: SAIOTEK
Code according to the funding entity: SA-2010/00057
Start-End date: 2010 - 2011 **Duration:** 2 years
Total amount: 54.188,03 €
- 22** **Name of the project:** Avances en Química Cuántica y su aplicación a problemas seleccionados de nanotecnología y bioquímica
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National

**Degree of contribution:** Researcher**Entity where project took place:** Universidad del País Vasco **Type of entity:** University**Name principal investigator (PI, Co-PI....):** Jesus M. Ugalde Uribe-Etxebarria**Funding entity or bodies:**

Ministerio de Ciencia e Innovación

Type of entity: Gobierno Estado**City funding entity:** Madrid, Community of Madrid, Spain**Type of participation:** Others**Code according to the funding entity:** CTQ200895739/BQU**Start-End date:** 2008 - 2011**Duration:** 4 years**Total amount:** 181.999,99 €**23 Name of the project:** Nanopartículas semiconductoras en entorno biológico: ¿aplicaciones biomédicas?**Type of project:** Basic research (including archaeological digs, etc)**Geographical area:** Regional**Degree of contribution:** Researcher**Entity where project took place:** Universidad del País Vasco **Type of entity:** University**Name principal investigator (PI, Co-PI....):** Jesus M. Ugalde Uribe-Etxebarria**Funding entity or bodies:**

Departamento de Industria. Gobierno Vasco

Type of entity: Gobierno Vasco**City funding entity:** Basque Country, Spain**Type of participation:** Others**Name of the programme:** SAIOTEK**Code according to the funding entity:** S-PC9UN02**Start-End date:** 2009 - 2010**Duration:** 2 years**Total amount:** 62.875,13 €**24 Name of the project:** Ensamblado de Nanoclusters: desarrollo de nuevos materiales semiconductores y magnéticos nanoporosos**Type of project:** Basic research (including archaeological digs, etc)**Geographical area:** Regional**Degree of contribution:** Researcher**Entity where project took place:** Universidad del País Vasco **Type of entity:** University**Name principal investigator (PI, Co-PI....):** Jesus M. Ugalde Uribe-Etxebarria**Funding entity or bodies:**

Departamento de Industria. Gobierno Vasco

Type of entity: Gobierno Vasco**City funding entity:** Basque Country, Spain**Type of participation:** Others**Name of the programme:** SAIOTEK**Start-End date:** 2007 - 2008**Duration:** 2 years**Total amount:** 45.000 €**25 Name of the project:** Ensamblado de Nanoclusters: desarrollo de nuevos materiales semiconductores**Type of project:** Basic research (including archaeological digs, etc)**Geographical area:** Regional**Degree of contribution:** Researcher**Entity where project took place:** Universidad del País Vasco **Type of entity:** University



Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria

Funding entity or bodies:

Departamento de Industria. Gobierno Vasco

Type of entity: Gobierno Vasco

City funding entity: Basque Country, Spain

Type of participation: Others

Name of the programme: SAIOTEK

Start-End date: 2006 - 2007

Duration: 3 years

Total amount: 35.000 €

26 Name of the project: Molecular modeling of lignin biosynthesis and degradation

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Suecia

Degree of contribution: Researcher

Entity where project took place: Örebro University **Type of entity:** University

City of entity: Örebro, Sweden

Name principal investigator (PI, Co-PI....): Leif A. Eriksson

Funding entity or bodies:

WURC (Wood Ultrastructure Research Center)

Type of entity: State agency

City funding entity: Sweden

Type of participation: Others

Start-End date: 2006 - 2006

Duration: 1 year

27 Name of the project: Properties and reactions of anthraquinones

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Suecia

Degree of contribution: Researcher

Entity where project took place: Örebro University **Type of entity:** University

City of entity: Örebro, Sweden

Name principal investigator (PI, Co-PI....): Leif A. Eriksson

Funding entity or bodies:

EKA Chemicals

Type of entity: Business

City funding entity: Sweden

Type of participation: Others

Start-End date: 2006 - 2006

Duration: 1 year

Total amount: 25.000 €

28 Name of the project: New Strategies for Photochemical Properties and Reactions in Pharmacology and Biomedicine

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Suecia

Degree of contribution: Researcher

Entity where project took place: Örebro University **Type of entity:** University

City of entity: Örebro, Sweden

Name principal investigator (PI, Co-PI....): Leif A. Eriksson

Funding entity or bodies:

National Science Research Center

Type of entity: State agency

City funding entity: Sweden

Type of participation: Others

Start-End date: 2005 - 2006

Duration: 2 years

Total amount: 39.600 €

29 Name of the project: Avances en Química Cuántica

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Current university student

Entity where project took place: Universidad del País Vasco

Type of entity: University

Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria

Funding entity or bodies:

Gobierno Vasco

Type of entity: Institución

City funding entity: Spain

Type of participation: Becario

Start-End date: 2001 - 2003

Duration: 3 years

30 Name of the project: Avances en Química Cuántica

Type of project: Basic research (including archaeological digs, etc)

Geographical area: National

Degree of contribution: Current university student

Entity where project took place: Universidad del País Vasco

Type of entity: University

Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria

Funding entity or bodies:

Gobierno Vasco

Type of entity: Institución

City funding entity: Spain

Type of participation: Becario

Start-End date: 2001 - 2003

Duration: 3 years

31 Name of the project: Investigación de nuevos materiales para el desarrollo de células solares de gran eficiencia

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Current university student

Entity where project took place: Universidad del País Vasco

Type of entity: University

Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria

Funding entity or bodies:

Universidad del País Vasco

Type of entity: University

City funding entity: Bilbao, Basque Country, Spain

Type of participation: Becario

Start-End date: 1999 - 2002

Duration: 4 years

32 Name of the project: Clusters de Metales de transición. Apantallamiento Electronico

Type of project: Basic research (including archaeological digs, etc)

Geographical area: Regional

Degree of contribution: Current university student

Entity where project took place: Universidad del País Vasco

Type of entity: University

City of entity: Donostia, Basque Country, Spain

Name principal investigator (PI, Co-PI....): Jesus M. Ugalde Uribe-Etxebarria

**Funding entity or bodies:**

Universidad del País Vasco

Type of entity: University**City funding entity:** Bilbao, Basque Country, Spain**Type of participation:** Becario**Start-End date:** 1998 - 2001**Duration:** 4 years

- 33 Name of the project:** Avances en el desarrollo y la aplicación de la química cuántica al estudio de moléculas con metales de transición

Type of project: Basic research (including archaeological digs, etc)**Geographical area:** National**Degree of contribution:** Current university student**Entity where project took place:** Universidad del País Vasco**Type of entity:** University**Name principal investigator (PI, Co-PI....):** Jesus M. Ugalde Uribe-Etxebarria**Funding entity or bodies:**

MINISTERIO DE EDUCACION Y CIENCIA

City funding entity: Spain**Type of participation:** Becario**Start-End date:** 1998 - 2000**Duration:** 2 years

- 34 Name of the project:** Estructura y propiedades de clusters con aplicaciones tecnológicas

Type of project: Basic research (including archaeological digs, etc)**Geographical area:** Regional**Degree of contribution:** Current university student**Entity where project took place:** Universidad del País Vasco**Type of entity:** University**Name principal investigator (PI, Co-PI....):** Jesus M. Ugalde Uribe-Etxebarria**Funding entity or bodies:**

Gobierno Vasco

Type of entity: Institución**City funding entity:** Spain**Type of participation:** Becario**Start-End date:** 1999 - 1999**Duration:** 1 year

Scientific and technological activities

Scientific production

H index: 24

Date of application: 31/12/2017

Publications, scientific and technical documents

- 1** Lorenzo Vallan; Esteban P. Urriolabeitia; Fernando Ruipérez; Jon M. Matxain; Ruben Canton Vitoria; Nikos Tagmatarchis; Ana M. Benito; Wolfgang K. Maser. Chirality-Induced Electron Spin Polarization and Enantiospecific Response in Solid-State Cross-Polarization Nuclear Magnetic Resonance. ACS Nano. 12, pp. 11426 - 11433. ACS, 27/11/2018. ISSN 0002-7863

Type of production: Scientific paper	Format: Journal
Position of signature: 4	Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 8	Corresponding author: No
Impact source: ISI	Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 13.709	Journal in the top 25%: Yes
Source of citations: WOS	Citations: 0
Relevant publication: Yes	
- 2** Lorenzo Vallan; Esteban P. Urriolabeitia; Fernando Ruipérez; Jon M. Matxain; Ruben Canton Vitoria; Nikos Tagmatarchis; Ana M. Benito; Wolfgang K. Maser. Supramolecular-enhanced charge-transfer within entangled polyamide chains as origin of the universal blue fluorescence of polymer carbon dots. Journal of the American Chemical Society. 140, pp. 12862 - 12869. ACS, 14/09/2018. Available on-line at: <<https://pubs.acs.org/doi/10.1021/jacs.8b06051>>. ISSN 0002-7863

DOI: 10.1021/jacs.8b06051

Type of production: Scientific paper	Format: Journal
Position of signature: 4	Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Total no. authors: 8	Corresponding author: No
Impact source: ISI	Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY
Impact index in year of publication: 14.357	Journal in the top 25%: Yes
Source of citations: WOS	Citations: 0
Relevant publication: Yes	
- 3** Ainara Erice; Alaitz Ruiz de Luzuriaga; Jon M. Matxain; Fernando Ruipérez; Jose M. Asua; Hans J. Grande; Alaitz Rekondo. Reprocessable and recyclable crosslinked poly(urea-urethane)s based on dynamic amine/urea exchange. Polymer. 145, pp. 127 - 136. Elsevier, 06/06/2018. Available on-line at: <<https://doi.org/10.1016/j.polymer.2018.04.076>>. ISSN 0032-3861

DOI: 10.1016/j.polymer.2018.04.076

Type of production: Scientific paper	Format: Journal
Position of signature: 3	

**Total no. authors:** 7**Impact source:** ISI**Impact index in year of publication:** 3.483**Source of citations:** WOS**Relevant publication:** Yes**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - POLYMER SCIENCE**Journal in the top 25%:** Yes**Citations:** 0

- 4** Jon Uranga; Jon Iñaki Mujika; Rafael Grande-Aztatzi; Jon M. Matxain. Oxidation of Acid, Base, and Amide Side-Chain Amino Acid Derivatives via Hydroxyl Radical. *Journal of Physical Chemistry B*. 122 - 19, pp. 4956 - 4971. American Chemical Society, 20/04/2018. Available on-line at: <<https://dx.doi.org/10.1021/acs.jpcc.7b12450>>. ISSN 1520-6106

DOI: 10.1021/acs.jpcc.7b12450**Type of production:** Scientific paper**Position of signature:** 4**Total no. authors:** 4**Impact source:** ISI**Impact index in year of publication:** 3.146**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** Yes**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** No**Citations:** 0

- 5** Fernando Ruipérez; Maialen Galdeano; Ekiñe Gimenez; Jon M. Matxain. Sulfenamides as Building Blocks for Efficient Disulfide-Based Self-Healing Materials. A Quantum Chemical Study. *ChemistryOpen*. 7 - 3, pp. 248 - 255. Wiley, 06/03/2018. Available on-line at: <<https://doi.org/10.1002/open.201800003>>. ISSN 2191-1363

DOI: 10.1002/open.201800003**Type of production:** Scientific paper**Position of signature:** 4**Total no. authors:** 4**Impact source:** ISI**Impact index in year of publication:** 2.801**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** Yes**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Journal in the top 25%:** No**Citations:** 0

- 6** Maude Desroches; Paula Mayorga Burrezo; Joël Boismenu Lavoie; Miriam Peña Alvarez; Carlos Gómez García; Jon M. Matxain; David Casanova; Jean-François Morin; Juan Casado. Breaking bonds, Forming Nanographene Diradicals with Pressure. *Angewandte Chemie. International Edition*. 56, pp. 16212 - 16217. Royal Society of Chemistry, 28/11/2017. ISSN 1433-7851

DOI: 10.1002/anie.201708740**Type of production:** Scientific paper**Position of signature:** 6**Total no. authors:** 9**Impact source:** ISI**Impact index in year of publication:** 11.994**Source of citations:** WOS**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Journal in the top 25%:** Yes**Citations:** 1

**Relevant publication:** Yes

- 7** Elena Formoso; Jon M. Matxain; Jose M. Asua; Fernando Ruiperez. The role of non-covalent interactions in the self-healing mechanism of disulfide-based polymers. *Physical Chemistry Chemical Physics*. 19, pp. 18461 - 18470. Royal Society of Chemistry, 01/07/2017. ISSN 1932-7447

DOI: 10.1039/C7CP03570E**Type of production:** Scientific paper**Position of signature:** 2**Total no. authors:** 4**Impact source:** ISI**Impact index in year of publication:** 3.906**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** Yes**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 1

- 8** Jon Uranga; Jon M. Matxain; Xabier Lopez; Jesus M. Ugalde; David Casanova Casas. Photosensitization mechanism of Cu(II) porphyrins. *Physical Chemistry Chemical Physics*. 19, pp. 20533. Royal Society of Chemistry, 29/06/2017. ISSN 1932-7447

DOI: 10.1039/C7CP03319B**Type of production:** Scientific paper**Position of signature:** 2**Total no. authors:** 5**Impact source:** ISI**Impact index in year of publication:** 3.906**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 1

- 9** Xiaowei An; Robert H. Aguirresarobe; Lourdes Irusta; Fernando Ruiperez; Jon M. Matxain; Xiangqiang Pan; Nora Aramburu; David Mecerreyes; Haritz Sardon; Jian Zhu. Aromatic diselenide crosslinkers to enhance the reprocessability and self-healing of polyurethane thermosets. *Polymer Chemistry*. 8, pp. 3641 - 3646. Royal Society of Chemistry, 22/05/2017. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2017/PY/C7PY00448F#ldivAbstract>>. ISSN 1932-7447

DOI: 10.1039/c7py00448f**Type of production:** Scientific paper**Position of signature:** 5**Total no. authors:** 10**Impact source:** ISI**Impact index in year of publication:** 4.927**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - POLYMER SCIENCE**Journal in the top 25%:** Yes**Citations:** 5

- 10** Jon Uranga Barandiaran; Oier Lakuntza Irigoien; Eloy Ramos Cordoba; Jon M. Matxain; Jon I. Mujika. A computational study of radical initiated protein backbone homolytic dissociation on all natural amino acids. *Physical Chemistry Chemical Physics*. 18, pp. 30972 - 30981. Royal Society of Chemistry, 18/10/2016. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b03210>>. ISSN 1932-7447

**DOI:** 10.1039/C6CP06529E**Type of production:** Scientific paper**Position of signature:** 4**Total no. authors:** 5**Impact source:** ISI**Impact index in year of publication:** 4.123**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 1

- 11** Alaitz Ruiz de Luzuriaga; Jon M. Matxain; Fernando Ruiperez; Roberto Martin; Jose M. Asua; German Cabañero; Ibon Odriozola. Transient mechanochromism in epoxy vitrimer composites containing aromatic disulfide crosslinks. Journal of Materials Chemistry C. 4, pp. 6220 - 6224. Royal Society of Chemistry, 08/06/2016. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2016/TC/C6TC02383E#divAbstract>>.

DOI: 10.1039/C6TC02383E**Type of production:** Scientific paper**Position of signature:** 2**Total no. authors:** 7**Impact source:** ISI**Impact index in year of publication:** 5.256**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - MATERIALS SCIENCE, MULTIDISCIPLINARY**Journal in the top 25%:** Yes**Citations:** 17

- 12** David Casanova; Jon M. Matxain; Jesus M. Ugalde. Plasmonic Resonances in the Al₁₃⁺ Cluster: Quantification and Origin of Exciton Collectivity. Journal of Physical Chemistry C. 120, pp. 12742 - 12750. American Chemical Society, 20/05/2016. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b03210>>. ISSN 1932-7447

DOI: 10.1021/acs.jpcc.6b03210**Type of production:** Scientific paper**Position of signature:** 2**Total no. authors:** 3**Impact source:** ISI**Impact index in year of publication:** 4.536**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** Yes**Citations:** 6

- 13** Rafael Grande Aztatz; Elena Formoso; Jose M. Mercero; Jon M. Matxain; Slawomir J. Grabowski; Jesus M. Ugalde. Structural and optical properties of the naked and passivated Al₅Au₅ bimetallic nanoclusters. JOURNAL OF CHEMICAL PHYSICS. 144, pp. 114302. American Institute of Physics, 15/03/2016. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/144/11/10.1063/1.4943129>>. ISSN 0021-9606

DOI: 10.1063/1.4943129**Type of production:** Scientific paper**Position of signature:** 4**Total no. authors:** 6**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** No

**Impact source:** ISI**Impact index in year of publication:** 2.965**Source of citations:** WOS**Relevant publication:** Yes**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** No**Citations:** 1

- 14** Jon M. Matxain; Jose M. Asua; Fernando Ruiperez. Design of new disulfide-based organic compounds for the improvement of self-healing materials. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 18, pp. 1758 - 1770. RSC, 01/2016. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2016/CP/C5CP06660C#!divAbstract>>. ISSN 1463-9076

DOI: 10.1039/C5CP06660C**Type of production:** Scientific paper**Position of signature:** 1**Total no. authors:** 3**Impact source:** ISI**Impact index in year of publication:** 4.123**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 23

- 15** Jon M. Azpiroz; Jon M. Matxain; Ivan Infante; Xabier Lopez; Jesus M. Ugalde. A DFT/TDDFT study on the optoelectronic properties of the amine-capped magic (CdSe)(13) nanocluster. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 15 - 26, pp. 10996 - 11005. RSC, 05/2013. Available on-line at: <<http://pubs.rsc.org/en/content/articlelanding/2013/cp/c3cp51687c#!divAbstract>>. ISSN 1463-9076

Type of production: Scientific paper**Position of signature:** 2**Impact source:** ISI**Impact index in year of publication:** 4.198**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** Yes**Citations:** 29

- 16** J. I. Mujika; J. Uranga; J. M. Matxain. Computational Study on the Attack of (OH)-O-center dot Radicals on Aromatic Amino Acids. CHEMISTRY-A EUROPEAN JOURNAL. 19 - 21, pp. 6862 - 6873. Wiley, 05/2013. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.201203862/abstract>>. ISSN 0947-6539

Type of production: Scientific paper**Position of signature:** 3**Impact source:** ISI**Impact index in year of publication:** 5.696**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Journal in the top 25%:** Yes**Citations:** 14

- 17** Jon M. Matxain; Fernando Ruiperez; Ivan Infante; Xabier Lopez; Jesus M. Ugalde; Gabriel Merino; Mario Piris. Communication: Chemical bonding in carbon dimer isovalent series from the natural orbital functional theory perspective. JOURNAL OF CHEMICAL PHYSICS. 138 - 15, pp. 151102. AIP, 04/2013. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/138/15/10.1063/1.4802585>>. ISSN 0021-9606
Type of production: Scientific paper
Position of signature: 1
Impact source: ISI
Impact index in year of publication: 3.122
Source of citations: WOS
Relevant publication: Yes
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 24
- 18** F. Ruiperez; M. Piris; J. M. Ugalde; J. M. Matxain. The natural orbital functional theory of the bonding in Cr-2, Mo-2 and W-2. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 15 - 6, pp. 2055 - 2062. RSC, 01/2013. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2013/CP/C2CP43559D#!divAbstract>>. ISSN 1463-9076
Type of production: Scientific paper
Position of signature: 4
Impact source: ISI
Impact index in year of publication: 4.198
Source of citations: WOS
Relevant publication: Yes
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: Yes
Citations: 22
- 19** Xabier Lopez; Fernando Ruiperez; Mario Piris; Jon M. Matxain; Eduard Matito; Jesus M. Ugalde. Performance of PNOF5 Natural Orbital Functional for Radical Formation Reactions: Hydrogen Atom Abstraction and C-C and O-O Homolytic Bond Cleavage in Selected Molecules. JOURNAL OF CHEMICAL THEORY AND COMPUTATION. 8 - 8, pp. 2646 - 2652. ACS Publications, 08/2012. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/ct300414t>>. ISSN 1549-9618
Type of production: Scientific paper
Position of signature: 4
Impact source: ISI
Impact index in year of publication: 5.389
Source of citations: WOS
Relevant publication: Yes
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: Yes
Citations: 20
- 20** M. Piris; X. Lopez; F. Ruiperez; J. M. Matxain; J. M. Ugalde. A natural orbital functional for multiconfigurational states. JOURNAL OF CHEMICAL PHYSICS. 134 - 16, pp. 164102. AIP, 04/2011. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/134/16/10.1063/1.3582792>>. ISSN 0021-9606
Type of production: Scientific paper
Position of signature: 4
Impact source: ISI
Impact index in year of publication: 3.333
Source of citations: WOS
Relevant publication: Yes
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 65

- 21** J. M. Matxain; M. Piris; F. Ruiperez; X. Lopez; J. M. Ugalde. Homolytic molecular dissociation in natural orbital functional theory. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 13 - 45, pp. 20129 - 20135. RSC, 2011. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2011/CP/c1cp21696a#!divAbstract>>. ISSN 1463-9076
- Type of production:** Scientific paper
Position of signature: 1
- Impact source:** ISI
- Impact index in year of publication:** 3.573
- Source of citations:** WOS
- Relevant results:** Portada del número
Relevant publication: Yes
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 24
- 22** M. Piris; J. M. Matxain; X. Lopez; J. M. Ugalde. Communication: The role of the positivity N-representability conditions in natural orbital functional theory. JOURNAL OF CHEMICAL PHYSICS. 133 - 11, pp. 111101. AIP, 09/2010. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/133/11/10.1063/1.3481578>>. ISSN 0021-9606
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
- Impact index in year of publication:** 2.920
- Source of citations:** WOS
- Relevant publication:** Yes
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 40
- 23** M. Piris; J. M. Matxain; X. Lopez; J. M. Ugalde. Communications: Accurate description of atoms and molecules by natural orbital functional theory. JOURNAL OF CHEMICAL PHYSICS. 132 - 3, pp. 031103. AIP, 01/2010. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/132/3/10.1063/1.3298694>>. ISSN 0021-9606
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
- Impact index in year of publication:** 2.921
- Source of citations:** WOS
- Relevant publication:** Yes
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 44
- 24** X. Lopez; M. Piris; J. M. Matxain; J. M. Ugalde. {Performance of PNOF3 for reactivity studies: X[BO] and X[CN] isomerization reactions (X = H, Li) as a case study}. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 12 - 40, pp. 12931 - 12934. RSC, 2010. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2010/CP/c003379k#!divAbstract>>. ISSN 1463-9076
- Type of production:** Scientific paper
Position of signature: 3
- Impact source:** ISI
- Impact index in year of publication:** 3.453
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes

**Source of citations:** WOS**Citations:** 14**Relevant results:** Portada del número**Relevant publication:** Yes

- 25** Jon M. Matxain; Daniel Padro; Mikael Ristila; Ake Strid; Leif A. Eriksson. Evidence of High center dot OH Radical Quenching Efficiency by Vitamin B-6. JOURNAL OF PHYSICAL CHEMISTRY B. 113 - 29, pp. 9629 - 9632. ACS Publications, 07/2009. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp903023c>>. ISSN 1520-6106

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - CHEMISTRY, PHYSICAL**Impact index in year of publication:** 3.471**Journal in the top 25%:** No**Source of citations:** WOS**Citations:** 31**Relevant publication:** Yes

- 26** M. Piris; J. M. Matxain; X. Lopez; J. M. Ugalde. Spin conserving natural orbital functional theory. JOURNAL OF CHEMICAL PHYSICS. 131 - 2, AIP, 07/2009. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/131/2/10.1063/1.3180958>>. ISSN 0021-9606

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Impact index in year of publication:** 3.093**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 31**Relevant publication:** Yes

- 27** Jose M. Mercero; Mario Piris; Jon M. Matxain; Xabier Lopez; Jesus M. Ugalde. Sandwich Complexes of the Metalloaromatic eta(3)-Al3R3 Ligand. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. 131 - 20, pp. 6949 - 6951. ACS Publications, 05/2009. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/ja8095043>>. ISSN 0002-7863

Type of production: Scientific paper**Format:** Journal**Position of signature:** 3**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Impact index in year of publication:** 8.580**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 11**Relevant publication:** Yes

- 28** Jon M. Matxain; Mario Piris; Xabier Lopez; Jesus M. Ugaide. Thermally Stable Solids Based on Endohedrally Doped ZnS Clusters. CHEMISTRY-A EUROPEAN JOURNAL. 15 - 20, pp. 5138 - 5144. Wiley, 2009. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.200802472/abstract>>. ISSN 0947-6539

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY

**Impact index in year of publication:** 5.382**Source of citations:** WOS**Relevant publication:** Yes**Journal in the top 25%:** Yes**Citations:** 11

- 29** J. M. Matxain; L. A. Eriksson; J. M. Mercero; X. Lopez; M. Piris; J. M. Ugalde; J. Poater; E. Matito; M. Sola. New solids based on B12N12 fullerenes. JOURNAL OF PHYSICAL CHEMISTRY C. 111 - 36, pp. 13354 - 13360. ACS Publications, 09/2007. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp073773j>>. ISSN 1932-7447

Type of production: Scientific paper**Position of signature:** 1**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 3.396**Source of citations:** WOS**Citations:** 25**Relevant publication:** Yes

- 30** Klefah A. K. Musa; Jon M. Matxain; Leif A. Eriksson. Mechanism of photoinduced decomposition of ketoprofen. JOURNAL OF MEDICINAL CHEMISTRY. 50 - 8, pp. 1735 - 1743. ACS Publications, 04/2007. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jm060697k>>. ISSN 0022-2623

Type of production: Scientific paper**Position of signature:** 2**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, MEDICINAL**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 5.115**Source of citations:** WOS**Citations:** 38**Relevant publication:** Yes

- 31** Jon M. Matxain; Mikael Ristilla; Ake Strid; Leif A. Eriksson. Theoretical study of the reaction of vitamin B-6 with O-1(2). CHEMISTRY-A EUROPEAN JOURNAL. 13 - 16, pp. 4636 - 4642. Wiley, 2007. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.200700002/abstract>>. ISSN 0947-6539

Type of production: Scientific paper**Position of signature:** 1**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 5.015**Source of citations:** WOS**Citations:** 31**Relevant publication:** Yes

- 32** Jon M. Matxain; Leif A. Eriksson; Jose M. Mercero; Jesus M. Ugalde; Eleonora Spano; Said Hamad; C. Richard A. Catlow. Electronic excitation energies of ZnSi nanoparticles. NANOTECHNOLOGY. 17 - 16, pp. 4100 - 4105. IOP Science, 08/2006. Available on-line at: <<http://iopscience.iop.org/0957-4484/17/16/018/>>. ISSN 0957-4484

Type of production: Scientific paper**Position of signature:** 1**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - NANOSCIENCE & NANOTECHNOLOGY**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 3.037**Source of citations:** WOS**Citations:** 15



Relevant publication: Yes

- 33** JM Mercero; JM Matxain; X Lopez; DM York; A Largo; LA Eriksson; JM Ugalde. Theoretical methods that help understanding the structure and reactivity of gas phase ions. INTERNATIONAL JOURNAL OF MASS SPECTROMETRY. 240 - 1, pp. 37 - 99. Elsevier, 01/2005. Available on-line at: <<http://www.sciencedirect.com/science/article/pii/S1387380604003744>>. ISSN 1387-3806

Type of production: Scientific paper

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 2.090

Source of citations: WOS

Relevant publication: Yes

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: No

Citations: 83

- 34** JM Mercero; JM Matxain; JM Ugalde. Mono- and multidecker sandwich-like complexes of the tetraazacyclobutadiene aromatic ring. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION. 43 - 41, pp. 5485 - 5488. Wiley, 2004. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/anie.200460498/abstract>>. ISSN 1433-7851

Type of production: Scientific paper

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 9.161

Source of citations: WOS

Relevant publication: Yes

Format: Journal

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

Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY

Journal in the top 25%: Yes

Citations: 38

- 35** JM Matxain; JM Ugalde; MD Towler; RJ Needs. Stability and aromaticity of BiNi rings and fullerenes. JOURNAL OF PHYSICAL CHEMISTRY A. 107 - 46, pp. 10004 - 10010. ACS Publications, 11/2003. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp036296n>>. ISSN 1089-5639

Type of production: Scientific paper

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 2.792

Source of citations: WOS

Relevant publication: Yes

Format: Journal

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

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: Yes

Citations: 37

- 36** JM Matxain; JM Mercero; JE Fowler; JM Ugalde. Electronic excitation energies of ZnO clusters. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. 125 - 31, pp. 9494 - 9499. ACS Publications, 08/2003. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/ja0264504>>. ISSN 0002-7863

Type of production: Scientific paper

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 6.516

Format: Journal

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

Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY

Journal in the top 25%: Yes

**Source of citations:** WOS**Citations:** 62**Relevant publication:** Yes

- 37** JM Matxain; JM Mercero; JE Fowler; JM Ugalde. Small clusters of group-(II-VI) materials: Zn_iX_i , $\text{X}=\text{Se}, \text{Te}$, $i=1-9$. PHYSICAL REVIEW A. 64 - 5, pp. 053201. APS Journals, 02/10/2001. Available on-line at: <http://journals.aps.org/pr/abstract/10.1103/PhysRevA.64.053201>. ISSN 1050-2947

DOI: 10.1103/PhysRevA.64.053201**Type of production:** Scientific paper**Position of signature:** 1**Impact source:** ISI**Impact index in year of publication:** 2.810**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 51

- 38** JM Matxain; A Irigoras; JE Fowler; JM Ugalde. Electronic excitation energies of ZnSi clusters. PHYSICAL REVIEW A. 64 - 1, pp. 013201. APS Journals, 13/06/2001. Available on-line at: <http://journals.aps.org/pr/abstract/10.1103/PhysRevA.64.013201>. ISSN 1050-2947

DOI: 10.1103/PhysRevA.64.013201**Type of production:** Scientific paper**Position of signature:** 1**Impact source:** ISI**Impact index in year of publication:** 2.810**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 51

- 39** JM Matxain; JE Fowler; JM Ugalde. Small clusters of II-VI materials: Zn_iO_i , $i=1-9$. PHYSICAL REVIEW A. 62 - 5, pp. 053201. APS Journals, 18/10/2000. Available on-line at: <http://journals.aps.org/pr/abstract/10.1103/PhysRevA.62.053201>. ISSN 1050-2947

Type of production: Scientific paper**Position of signature:** 1**Impact source:** ISI**Impact index in year of publication:** 2.831**Source of citations:** WOS**Relevant publication:** Yes**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Citations:** 66

- 40** JM Matxain; JE Fowler; JM Ugalde. Small clusters of II-VI materials: Zn_iSi_i , $i=1-9$. PHYSICAL REVIEW A. 61 - 5, pp. 053201. APS Journals, 14/04/2000. Available on-line at: <http://journals.aps.org/pr/abstract/10.1103/PhysRevA.61.053201>. ISSN 1050-2947

Type of production: Scientific paper**Position of signature:** 1**Impact source:** ISI**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

**Impact index in year of publication:** 2.831**Source of citations:** WOS**Relevant publication:** Yes**Journal in the top 25%:** Yes**Citations:** 55

- 41** Jon Uranga; Jon I. Mujika; Jon M. Matxain. ·OH Oxidation Towards S- and OH- Containing Amino Acids. *Journal of Physical Chemistry B*. 119, pp. 15430. ACS, 20/11/2015. Available on-line at: <http://pubs.acs.org/doi/10.1021/acs.jpcc.5b09825>. ISSN 1520-6106

DOI: 10.1021/acs.jpcc.5b09825**Type of production:** Scientific paper**Position of signature:** 3**Total no. authors:** 3**Impact source:** ISI**Impact index in year of publication:** 3.187**Source of citations:** WOS**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Corresponding author:** Yes**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** No**Citations:** 7

- 42** Elisa Jimenez Izal; Jon M. Azpiroz; Riti Gupta; Jon M. Matxain; Jesus M. Ugalde. CdS nanoclusters doped with divalent atoms. *Journal of Molecular Modeling*. 20, pp. 2227. Springer, 30/06/2014. Available on-line at: <http://link.springer.com/article/10.1007%2Fs00894-014-2227-3>. ISSN 1610-2940

Type of production: Scientific paper**Position of signature:** 4**Impact source:** ISI**Impact index in year of publication:** 1.736**Source of citations:** WOS**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Journal in the top 25%:** No**Citations:** 1

- 43** Elisa Jimenez Izal; Diego Moreno; Jose M. Mercero Larrazza; Jon M. Matxain Beraza; Martha Audiffred; Gabriel Merino; Jesus M. Ugalde Uribe-Etxebarria. Doped Aluminum Cluster Anions: Size Matters. *Journal of Physical Chemistry A*. 118 - 24, pp. 4309 - 4314. ACS Publishing, 19/05/2014. Available on-line at: <http://pubs.acs.org/doi/abs/10.1021/jp501496b>. ISSN 1089-5639

Type of production: Scientific paper**Position of signature:** 4**Impact source:** ISI**Impact index in year of publication:** 2.693**Source of citations:** WOS**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** No**Citations:** 4

- 44** M. Piris; F. Ruiperez; J. M. Matxain. Assessment of the second-order perturbative corrections to PNOF5. *MOLECULAR PHYSICS*. 112 - 5-6, SI, pp. 1 - 8. Taylor & Francis, 03/2014. Available on-line at: <http://www.tandfonline.com/doi/abs/10.1080/00268976.2013.854933#.VSZSMZSsXmE>. ISSN 0026-8976

Type of production: Scientific paper**Position of signature:** 3**Impact source:** ISI**Impact index in year of publication:** 1.720**Source of citations:** WOS**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** No**Citations:** 5

- 45** M. Piris; J. M. Matxain; X. Lopez. The intrapair electron correlation in natural orbital functional theory. JOURNAL OF CHEMICAL PHYSICS. 139 - 23, pp. 234109. AIP, 12/2013. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/139/23/10.1063/1.4844075>>. ISSN 0021-9606
Type of production: Scientific paper
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 3.122
Source of citations: WOS
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 27
- 46** Elisa Jimenez Izal; Jon M. Matxain Beraza; Mario Piris Silvera; Jesus M. Ugalde Uribe-Etxebarria. Second-Row Transition Metal doping of ZnSi (i=12,16) nanoclusters: Structural and Magnetic Properties. Computation. 1 - 3, pp. 31 - 45. MDPI, 14/11/2013. Available on-line at: <<http://www.mdpi.com/2079-3197/1/3/31>>. DOI: 10.3390/computation1030031
Type of production: Scientific paper
Position of signature: 2
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
- 47** Oier Lakuntza; Jon M. Matxain; Fernando Ruiperez; Jesus M. Ugalde; Peter B. Armentrout. Quantum Chemical Study of the Reactions between Pd+/Pt+ and H2O/H2S. CHEMISTRY-A EUROPEAN JOURNAL. 19 - 27, pp. 8832 - 8838. Wiley, 07/2013. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.201300222/abstract>>. ISSN 0947-6539
Type of production: Scientific paper
Position of signature: 2
Impact source: ISI
Impact index in year of publication: 5.696
Source of citations: WOS
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY
Journal in the top 25%: Yes
Citations: 1
- 48** Jon M. Matxain; Fernando Ruiperez; Mario Piris. Computational study of Be-2 using Piris natural orbital functionals. JOURNAL OF MOLECULAR MODELING. 19 - 5, pp. 1967 - 1972. Springer, 05/2013. Available on-line at: <<http://link.springer.com/article/10.1007%2Fs00894-012-1548-3>>. ISSN 1610-2940
Type of production: Scientific paper
Position of signature: 1
Impact source: ISI
Impact index in year of publication: 1.867
Source of citations: WOS
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY
Journal in the top 25%: No
Citations: 0
- 49** Jon I. Mujika; Jon M. Matxain. Theoretical study of the pH-dependent antioxidant properties of vitamin C. JOURNAL OF MOLECULAR MODELING. 19 - 5, pp. 1945 - 1952. Springer, 05/2013. Available on-line at: <<http://link.springer.com/article/10.1007%2Fs00894-012-1465-5>>. ISSN 1610-2940
Type of production: Scientific paper
Position of signature: 2
Format: Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee



Impact source: ISI

Impact index in year of publication: 1.867

Source of citations: WOS

Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY

Journal in the top 25%: No

Citations: 6

- 50** Mario Piris; Jon M. Matxain; Xabier Lopez; Jesus M. Ugalde. The one-electron picture in the Piris natural orbital functional 5 (PNOF5). THEORETICAL CHEMISTRY ACCOUNTS. 132 - 2, pp. 1298. Springer, 02/2013. Available on-line at: <<http://link.springer.com/article/10.1007%2Fs00214-012-1298-4>>. ISSN 1432-881X

DOI: 10.1007/s00214-012-1298-4

Type of production: Scientific paper

Position of signature: 2

Format: Journal

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

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: No

Impact source: ISI

Impact index in year of publication: 2.143

Source of citations: WOS

Citations: 19

- 51** Elisa Jimenez-Izal; Jon M. Matxain; Mario Piris; Jesus M. Ugalde. Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 14 - 27, pp. 9676 - 9682. RCS, 06/2012. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2012/CP/c2cp41273j#!divAbstract>>. ISSN 1463-9076

Type of production: Scientific paper

Position of signature: 2

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: Yes

Impact source: ISI

Impact index in year of publication: 3.829

Source of citations: WOS

Citations: 7

- 52** Jon M. Matxain; Mario Piris; Jon Uranga; Xabier Lopez; Gabriel Merino; Jesus M. Ugalde. The Nature of Chemical Bonds from PNOF5 Calculations. CHEMPHYSICHEM. 13 - 9, pp. 2297 - 2303. Wiley, 06/2012. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/cphc.201200205/abstract>>. ISSN 1439-4235

Type of production: Scientific paper

Position of signature: 1

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: Yes

Impact source: ISI

Impact index in year of publication: 3.349

Source of citations: WOS

Citations: 15

- 53** Mario Piris; Jon M. Matxain; Xabier Lopez; Jesus M. Ugalde. The extended Koopmans' theorem: Vertical ionization potentials from natural orbital functional theory. JOURNAL OF CHEMICAL PHYSICS. 136 - 17, pp. 174116. AIP, 05/2012. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/136/17/10.1063/1.4709769>>. ISSN 0021-9606

Type of production: Scientific paper

Position of signature: 2

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Impact source: ISI

Impact index in year of publication: 3.164**Source of citations:** WOS**Journal in the top 25%:** Yes**Citations:** 22

- 54** Jon M. Matxain; Mario Piris; Jose M. Mercero; Xabier Lopez; Jesus M. Ugalde. sp(3) Hybrid orbitals and ionization energies of methane from PNOF5. CHEMICAL PHYSICS LETTERS. 531, pp. 272 - 274. Elsevier, 04/2012. Available on-line at: <<http://www.sciencedirect.com/science/article/pii/S0009261412002291>>. ISSN 0009-2614

Type of production: Scientific paper**Position of signature:** 1**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** No**Impact source:** ISI**Impact index in year of publication:** 2.145**Source of citations:** WOS**Citations:** 13

- 55** O. Lakuntza; J. M. Matxain; F. Ruiperez; M. Besora; F. Maseras; J. M. Ugalde; M. Schlangen; H. Schwarz. {A computational study on the intriguing mechanisms of the gas-phase thermal activation of methane by bare $\{[Ni(H)(OH)](+)\}$. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 14 - 26, pp. 9306 - 9310. RSC, 02/2012. Available on-line at: <<http://pubs.rsc.org/en/Content/ArticleLanding/2012/CP/c2cp23502a#!divAbstract>>. ISSN 1463-9076

Type of production: Scientific paper**Position of signature:** 2**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 3.829**Source of citations:** WOS**Citations:** 7

- 56** Xabier Lopez; Mario Piris; Jon M. Matxain; Fernando Ruiperez; Jesus M. Ugalde. Natural Orbital Functional Theory and Reactivity Studies of Diradical Rearrangements: Ethylene Torsion as a Case Study. CHEMPHYSICHEM. 12 - 9, pp. 1673 - 1676. Wiley, 06/2011. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/cphc.201100190/abstract>>. ISSN 1439-4235

Type of production: Scientific paper**Position of signature:** 3**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Atomic and Molecular Physics, and Optics**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 3.412**Source of citations:** WOS**Citations:** 14

- 57** Xabier Lopez; Fernando Ruiperez; Mario Piris; Jon M. Matxain; Jesus M. Ugalde. Diradicals and Diradicaloids in Natural Orbital Functional Theory. CHEMPHYSICHEM. 12 - 6, pp. 1061 - 1065. Wiley, 04/2011. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/cphc.201100136/abstract>>. ISSN 1439-4235

Type of production: Scientific paper**Position of signature:** 4**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Atomic and Molecular Physics, and Optics**Journal in the top 25%:** Yes**Impact source:** ISI**Impact index in year of publication:** 3.412**Source of citations:** WOS**Citations:** 19

- 58** Elisa Jimenez-Izal; Jon M. Matxain; Mario Piris; Jesus M. Ugalde. Thermal Stability of Endohedral First-Row Transition-Metal TM@ZnSi Structures, $i=12, 16$. JOURNAL OF PHYSICAL CHEMISTRY C. 115 - 16, pp. 7829 - 7835. ACS Publishing, 04/2011. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp108640w>>. ISSN 1932-7447
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
- Impact index in year of publication:** 4.805
- Source of citations:** WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - MATERIALS SCIENCE, MULTIDISCIPLINARY
Journal in the top 25%: Yes
Citations: 2
- 59** Elixabete Rezabal; Juergen Gauss; Jon M. Matxain; Robert Berger; Martin Diefenbach; Max C. Holthausen. Quantum chemical assessment of the binding energy of CuO⁺. JOURNAL OF CHEMICAL PHYSICS. 134 - 6, pp. 064304. AIP, 02/2011. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/134/6/10.1063/1.3537797>>. ISSN 0021-9606
- Type of production:** Scientific paper
Position of signature: 3
- Impact source:** ISI
- Impact index in year of publication:** 3.333
- Source of citations:** WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 14
- 60** J. M. Matxain; M. Piris; X. Lopez; J. M. Ugalde. Complete basis set limit extrapolation calculations with PNOF3. CHEMICAL PHYSICS LETTERS. 499 - 1-3, pp. 164 - 167. Elsevier, 10/2010. Available on-line at: <<http://www.sciencedirect.com/science/article/pii/S0009261410012145>>. ISSN 0009-2614
- Type of production:** Scientific paper
Position of signature: 1
- Impact source:** ISI
- Impact index in year of publication:** 2.280
- Source of citations:** WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: No
Citations: 10
- 61** Oier Lakuntza; Jon M. Matxain; Jesus M. Ugalde. Quantum Chemical Study of the Reaction between Ni⁺ and H₂S. CHEMPHYSCHEM. 11 - 14, pp. 3172 - 3178. Wiley, 10/2010. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/cphc.200901020/abstract>>. ISSN 1439-4235
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
- Impact index in year of publication:** 3.339
- Source of citations:** WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 3
- 62** Elena Formoso; Jon M. Matxain; Xabier Lopez; Darrin M. York. Molecular Dynamics Simulation of Bovine Pancreatic Ribonuclease A-CpA and Transition State-like Complexes. JOURNAL OF PHYSICAL CHEMISTRY B. 114 - 21, pp. 7371 - 7382. ACS Publications, 06/2010. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp909004y>>. ISSN 1520-6106



Type of production: Scientific paper

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 3.603

Source of citations: WOS

Format: Journal

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

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: No

Citations: 12

- 63** Jon M. Matxain; Elixabete Rezabal; Xabier Lopez; Jesus M. Ugalde; Laura Gagliardi. Erratum: Quantum Monte Carlo study of the ground state and low-lying excited states of the scandium dimer (vol 128, 194315, 2008). JOURNAL OF CHEMICAL PHYSICS. 132 - 13, pp. 139901. AIP, 04/2010. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/132/13/10.1063/1.3372793>>. ISSN 0021-9606

Type of production: Scientific paper

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 2.920

Source of citations: WOS

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: Yes

Citations: 6

- 64** Elisa Jimenez-Izal; Jon M. Matxain; Mario Piris; Jesus M. Ugalde. Structure and Stability of the Endohedrally Doped (X@C_{di}Si)(i=4,9,12,15,16)(q=0,+/- 1), X = Na, K, Cl, Br, Nanoclusters. JOURNAL OF PHYSICAL CHEMISTRY C. 114 - 6, pp. 2476 - 2483. ACS Publishing, 02/2010. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp909357c>>. ISSN 1932-7447

Type of production: Scientific paper

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 4.524

Source of citations: WOS

Format: Journal

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

Category: Science Edition - NANOSCIENCE & NANOTECHNOLOGY

Journal in the top 25%: Yes

Citations: 6

- 65** M. Piris; J. M. Matxain; J. M. Ugalde. Piris natural orbital functional study of the dissociation of the radical helium dimer. JOURNAL OF CHEMICAL PHYSICS. 129 - 1, 07/2008. ISSN 0021-9606

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 3.166

Source of citations: WOS

Format: Journal

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: Yes

Citations: 15

- 66** Jon M. Matxain; Elixabete Rezabal; Xabier Lopez; Jesus M. Ugalde; Laura Gagliardi. Quantum Monte Carlo study of the ground state and low-lying excited states of the scandium dimer. JOURNAL OF CHEMICAL PHYSICS. 128 - 19, pp. 194315. AIP, 05/2008. Available on-line at: <<http://scitation.aip.org/content/aip/journal/jcp/128/19/10.1063/1.2920480>>. ISSN 0021-9606

Type of production: Scientific paper

Position of signature: 1

Impact source: ISI

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Impact index in year of publication: 3.166**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 11

- 67** Jon M. Matxain; Elena Formoso; Jose M. Mercero; Mario Piris; Xabier Lopez; Jesus M. Ugalde. Magnetic Endohedral Transition-Metal-Doped Semiconducting-Nanoclusters. CHEMISTRY-A EUROPEAN JOURNAL. 14 - 28, pp. 8547 - 8554. Wiley, 2008. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.200800376/abstract>>. ISSN 0947-6539

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - CHEMISTRY, MULTIDISCIPLINARY**Impact index in year of publication:** 5.454**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 5

- 68** Jon M. Matxain; Mario Piris; Elena Formoso; Jose M. Mercero; Xabier Lopez; Jesus M. Ugalde. Endohedral stannaspherenes Mn@Sn-12 and its dimer: Ferromagnetic or antiferromagnetic?. CHEMPHYSICHEM. 8 - 14, pp. 2096 - 2099. Wiley, 10/2007. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/cphc.200700428/abstract>>. ISSN 1439-4235

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - CHEMISTRY, PHYSICAL**Impact index in year of publication:** 3.449**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 16

- 69** Eider San Sebastian; Jon M. Matxain; Leif A. Eriksson; Roland H. Stote; Annick Dejaegere; Fernando P. Cossio; Xabier Lopez. Metal ion dependent adhesion sites in integrins: A combined DFT and QMC study on Mn²⁺. JOURNAL OF PHYSICAL CHEMISTRY B. 111 - 30, pp. 9099 - 9103. ACS Publications, 08/2007. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp071065s>>. ISSN 1520-6106

Type of production: Scientific paper**Format:** Journal**Position of signature:** 2**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - CHEMISTRY, PHYSICAL**Impact index in year of publication:** 4.115**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 1

- 70** Jon M. Matxain; Leif A. Eriksson; Elena Formoso; Mario Piris; Jesus M. Ugalde. Endohedral (X@ZnSi)(i=)(0,+/-)(4-16) nanoclusters, X = Li, Na, K, Cl, Br. JOURNAL OF PHYSICAL CHEMISTRY C. 111 - 9, pp. 3560 - 3565. ACS Publications, 03/2007. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp0668697>>. ISSN 1932-7447

Type of production: Scientific paper**Format:** Journal**Position of signature:** 1**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Impact source:** ISI**Category:** Science Edition - NANOSCIENCE & NANOTECHNOLOGY**Impact index in year of publication:** 3.396**Journal in the top 25%:** Yes**Source of citations:** WOS**Citations:** 10

- 71** Jon M. Matxain; Mikael Ristila; Ake Strid; Leif A. Eriksson. Theoretical study of the antioxidant properties of pyridoxine. JOURNAL OF PHYSICAL CHEMISTRY A. 110 - 48, pp. 13068 - 13072. ACS Publications, 12/2006. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp065115p>>. ISSN 1089-5639
- Type of production:** Scientific paper
Position of signature: 1
- Impact source:** ISI
Impact index in year of publication: 3.047
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: Yes
Citations: 38
- 72** Jon I. Mujika; Jon M. Matxain; Leif A. Eriksson; Xabier Lopez. Resonance structures of the amide bond: The advantages of planarity. CHEMISTRY-A EUROPEAN JOURNAL. 12 - 27, pp. 7215 - 7224. Wiley, 09/2006. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.200600052/abstract>>. ISSN 0947-6539
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
Impact index in year of publication: 5.015
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY
Journal in the top 25%: Yes
Citations: 30
- 73** Mikael Ristila; Jon M. Matxain; Ake Strid; Leif A. Eriksson. pH-dependent electronic and spectroscopic properties of pyridoxine (vitamin B-6). JOURNAL OF PHYSICAL CHEMISTRY B. 110 - 33, pp. 16774 - 16780. ACS Publications, 08/2006. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp062800n>>. ISSN 1520-6106
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
Impact index in year of publication: 4.115
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: Yes
Citations: 23
- 74** JM Mercero; E Formoso; JM Matxain; LA Eriksson; JM Ugalde. {Sandwich complexes based on the ``All-Metal{''} Al-4(2-) aromatic ring}. CHEMISTRY-A EUROPEAN JOURNAL. 12 - 17, pp. 4495 - 4502. Wiley, 06/2006. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/chem.200600106/abstract>>. ISSN 0947-6539
- Type of production:** Scientific paper
Position of signature: 3
- Impact source:** ISI
Impact index in year of publication: 5.015
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY
Journal in the top 25%: Yes
Citations: 28
- 75** S Hamad; CRA Catlow; E Spano; JM Matxain; JM Ugalde. Structure and properties of ZnS nanoclusters. JOURNAL OF PHYSICAL CHEMISTRY B. 109 - 7, pp. 2703 - 2709. ACS Publications, 02/2005. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp0465940>>. ISSN 1520-6106
- Type of production:** Scientific paper
Position of signature: 4
- Format:** Journal



Impact source: ISI

Impact index in year of publication: 4.033

Source of citations: WOS

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

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: Yes

Citations: 88

- 76** JM Matxain; JM Mercero; A Irigoras; JM Ugalde. Discordant results on the $\text{FeO}^{++}\text{H}_2$ reaction reconciled by quantum Monte Carlo theory. MOLECULAR PHYSICS. 102 - 23-24, pp. 2635 - 2637. Taylor & Francis, 12/2004. Available on-line at: <<http://dx.doi.org/10.1080/00268970412331292768>>. ISSN 0026-8976

Type of production: Scientific paper

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 1.406

Source of citations: WOS

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: No

Citations: 15

- 77** JM Matxain; JM Mercero; JE Fowler; JM Ugalde. Clusters of II-VI materials: CdiX_i , $X = \text{S, Se, Te}$, $i \leq 16$. JOURNAL OF PHYSICAL CHEMISTRY A. 108 - 47, pp. 10502 - 10508. ACS Publications, 11/2004. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp037195s>>. ISSN 1089-5639

Type of production: Scientific paper

Position of signature: 1

Impact source: ISI

Impact index in year of publication: 2.639

Source of citations: WOS

Format: Journal

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

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: No

Citations: 41

- 78** JM Mercero; JM Matxain; E Rezabal; X Lopez; JM Ugalde. The first solvation shell of aluminum(III) and magnesium(II) cations in a protein model environment. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 98 - 4, pp. 409 - 424. Wiley, 06/2004. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/qua.20075/abstract>>. ISSN 0020-7608

Type of production: Scientific paper

Position of signature: 2

Impact source: ISI

Impact index in year of publication: 1.392

Source of citations: WOS

Format: Journal

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

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: No

Citations: 18

- 79** JM Mercero; JI Mujika; JM Matxain; X Lopez; JM Ugalde. Incremental binding free energies of aluminum (III) vs. magnesium (II) complexes. CHEMICAL PHYSICS. 295 - 2, pp. 175 - 184. Elsevier, 12/2003. Available on-line at: <<http://www.sciencedirect.com/science/article/pii/S0301010403004221>>. ISSN 0301-0104

Type of production: Scientific paper

Position of signature: 3

Impact source: ISI

Impact index in year of publication: 2.070

Source of citations: WOS

Format: Journal

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

Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: No

Citations: 10

- 80** JM Matxain; JM Mercero; JE Fowler; JM Ugalde. Clusters of group II-VI materials: CdiOi ($i \leq 15$). JOURNAL OF PHYSICAL CHEMISTRY A. 107 - 46, pp. 9918 - 9923. ACS Publications, 11/2003. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp035226d>>. ISSN 1089-5639
- Type of production:** Scientific paper
Position of signature: 1
- Impact source:** ISI
Impact index in year of publication: 2.792
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: Yes
Citations: 17
- 81** RP Diez; JA Alonso; JM Matxain; JM Ugalde. Electronic metastable bound states of Mn-2(2+) and Co-2(2+). CHEMICAL PHYSICS LETTERS. 372 - 1-2, pp. 82 - 89. Elsevier, 22/04/2003. Available on-line at: <<http://www.sciencedirect.com/science/article/pii/S0009261403003658>>. ISSN 0009-2614
- Type of production:** Scientific paper
Position of signature: 3
- Impact source:** ISI
Impact index in year of publication: 2.438
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 6
- 82** JM Mercero; JM Matxain; X Lopez; JE Fowler; JM Ugalde. Aluminum (III) interactions with the side chains of aromatic aminoacids. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 90 - 2, pp. 859 - 881. Wiley, 10/2002. Available on-line at: <<http://onlinelibrary.wiley.com/doi/10.1002/qua.952/abstract;jsessionid=45DC85438A9D65C42191726061E2F58C.f04t04>>. ISSN 0020-7608
- Type of production:** Scientific paper
Position of signature: 2
- Impact source:** ISI
Impact index in year of publication: 1.514
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: No
Citations: 13
- 83** JM Matxain; A Irigoras; JE Fowler; JM Ugalde. Electronic excitation energies of small ZnSi clusters. PHYSICAL REVIEW A. 63 - 1, pp. 013202. APS Journals, 11/12/2000. Available on-line at: <<http://journals.aps.org/pr/abstract/10.1103/PhysRevA.63.013202>>. ISSN 1050-2947
- Type of production:** Scientific paper
Position of signature: 1
- Impact source:** ISI
Impact index in year of publication: 2.810
Source of citations: WOS
- Format:** Journal
Degree of contribution: Author or co-author of article in journal with external admissions assessment committee
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
Citations: 3
- 84** J van de Bovenkamp; JM Matxain; FB van Duijneveldt; T Steiner. Combined ab initio computational and statistical investigation of a model C-H center dot center dot center dot O hydrogen bonded dimer as occurring in 1,4-benzoquinone. JOURNAL OF PHYSICAL CHEMISTRY A. 103 - 15, pp. 2784 - 2792. ACS Publications, 04/1999. Available on-line at: <<http://pubs.acs.org/doi/abs/10.1021/jp983607z>>. ISSN 1089-5639

**Type of production:** Scientific paper**Position of signature:** 2**Impact source:** ISI**Impact index in year of publication:** 2.695**Source of citations:** WOS**Format:** Journal**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee**Category:** Science Edition - CHEMISTRY, PHYSICAL**Journal in the top 25%:** Yes**Citations:** 21

- 85** Elisa Jimenez Izal; Jesus M. Ugalde; Jon M. Matxain. Nanocluster-Assembled Materials. Computational Modeling of Inorganic Nanomaterials. 4, pp. 113 - 148. CRC Press, Taylor & Francis Group, 01/03/2016. ISBN 9781466576414

Type of production: Book chapter**Position of signature:** 3**Total no. authors:** 3**Format:** Book**Degree of contribution:** Author or co-author of chapter in book**Corresponding author:** Yes

- 86** The one-electron picture in the Pirs Natural Orbital Functional 5 (PNOF5). 8TH CONGRESS ON ELECTRONIC STRUCTURE: PRINCIPLES AND APPLICATIONS (ESPA 2012): A CONFERENCE SELECTION FROM THEORETICAL CHEMISTRY ACCOUNTS. 5, pp. 5. Springer, 05/2014. ISBN 978-3-642-41271-4

Collection: Highlights in Theoretical Chemistry**Type of production:** Book chapter**Position of signature:** 2**Degree of contribution:** Author or co-author of article in journal with external admissions assessment committee

- 87** Jon M. Matxain Beraza. Small Clusters of II-VI Materials. UPV/EHU, 04/03/2003. ISBN 84-8373-461-3

Type of production: Scientific book or monograph**Position of signature:** 1**Relevant publication:** Yes**Format:** Book**Degree of contribution:** Author or co-author of entire book

Works submitted to national or international conferences

- 1** **Title of the work:** Theoretical Self-Healing Capacity of Polymers with Disulfide Cross-links
Name of the conference: 2nd International Caparica Christmas Congress on Translational Chemistry
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Lisboa, Portugal
Date of event: 04/12/2017
End date: 07/12/2017
Organising entity: Universidade Nova de Lisboa
Jon M. Matxain.
- 2** **Title of the work:** Transition Metal Doped Magnetic Zn₁₂S₁₂ Nanoparticles
Name of the conference: 11th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2017)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote talk
City of event: Munich, Germany
Date of event: 26/08/2017
End date: 01/09/2017
Organising entity: Asociación Mundial de Químicos Teóricos (WATOC)



Jon M. Matxain.

- 3** **Title of the work:** Magnetic endohedral TM@Zn₁₂S₁₂ nanoclusters: A predictive work
Name of the conference: From Bioinorganic Chemistry to Catalysis
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - invited/keynote talk
City of event: Donostia, Spain
Date of event: 06/06/2017
End date: 06/06/2017
Organising entity: Donostia International Physics Center
Type of entity: Centro de Investigación
Jon M. Matxain.
- 4** **Title of the work:** Computational Chemistry Applied to: Nanoclusters, Polymers and Biochemistry
Name of the conference: Transborder Theoretical Chemistry Days
Type of event: Conference **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk
City of event: Burdeos, France
Date of event: 09/11/2016
End date: 10/11/2016
Organising entity: University of Bordeaux
Type of entity: University
Jon M. Matxain.
- 5** **Title of the work:** Disulfide-based organic compounds for the design of improved self-healing materials
Name of the conference: Energy, Materials and Nanotechnology Meeting (EMN Theory)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Las Vegas, United States of America
Date of event: 10/10/2016
End date: 14/10/2016
Organising entity: EMN
Type of entity: Business
Jon M. Matxain.
- 6** **Title of the work:** Aluminum and Aluminum-Gold Nanoparticles
Name of the conference: 10th conference on Electronic Structure: Principles and Applications (ESPA)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Castelló, Spain
Date of event: 28/06/2016
End date: 01/07/2016
Organising entity: Universitat Jaume I
Jon M. Matxain.
- 7** **Title of the work:** IPolymorphs. Novel Routes to Inorganic Polymorphs
Name of the conference: IPolymorphs. Novel Routes to Inorganic Polymorphs
Type of event: Conference **Geographical area:** Internacional
Type of participation: Organizational - President of Committee
City of event: Donostia, Spain
Date of event: 28/06/2016
End date: 01/07/2016
Type of entity: Centro de Investigación



Organising entity: Donostia International Physics Center
Jon M. Matxain.

8 Title of the work: Disulfide-based organic compounds for the design of improved self-healing materials

Name of the conference: 251st American Chemistry Society National Meeting

Type of event: Conference

Geographical area: Non EU International

Type of participation: 'Participatory - poster

City of event: San Diego, United States of America

Date of event: 13/03/2016

End date: 17/03/2016

Organising entity: Amecan Chemical Society

Type of entity: Associations and Groups

Jon M. Matxain.

9 Title of the work: Attack of OH radical to the OH- and S- containing amino acids

Name of the conference: Theoretical Biophysics 2015 (Theobio 15)

Type of event: Conference

Geographical area: Internacional

Type of participation: 'Participatory - poster

City of event: Cagliari, Italy

Date of event: 08/06/2015

End date: 12/06/2015

Organising entity: Universidad de Cagliari

Type of entity: University

Jon M. Matxain.

10 Title of the work: Novel Solid Polymorphs by self assembling of nanoclusters

Name of the conference: ImagineNano2015

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - invited/keynote talk

City of event: Bilbao, Basque Country, Spain

Date of event: 10/03/2015

End date: 13/03/2014

Organising entity: Donostia International Physics Center

Type of entity: Centro de Investigación

Jon M. Matxain.

11 Title of the work: Novel Solid Polymorphs by self assembling of nanoclusters

Name of the conference: 10th Triennial congress of the World Association of Theoretical and Computational Chemists. WATOC 2014

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - invited/keynote talk

City of event: Santiago de Compostela, Galicia, Spain

Date of event: 05/10/2014

End date: 10/10/2014

Organising entity: Asociación Mundial de Químicos Teóricos y Computacionales (WATOC)

Type of entity: Associations and Groups

Jon M. Matxain.

12 Title of the work: Nanocluster assembled materials

Name of the conference: Materials Science 2013

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - invited/keynote talk



City of event: Las Vegas, United States of America

Date of event: 07/10/2013

End date: 09/10/2013

Organising entity: OMICS group

Jon M. Matxain.

Type of entity: Grupo Editorial

13 Title of the work: Study of the attack of OH radicals on aromatic amino acids

Name of the conference: Theoretical Biophysics 2013 (Theobio 13)

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - invited/keynote talk

City of event: Gotteborg, Sweden

Date of event: 24/06/2013

End date: 27/06/2013

Organising entity: Universidad de Gotteborg

Jon M. Matxain.

Type of entity: University

14 Title of the work: Nature of chemical bonds by means of PNOF theory

Name of the conference: Congreso de Químicos Teóricos de expresión latina (QUITEL 2011)

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - invited/keynote talk

City of event: Riviera Maya, Mexico

Date of event: 04/12/2011

End date: 09/12/2011

Organising entity: CINVESTAV

Jon M. Matxain.

Type of entity: R&D Centre

15 Title of the work: Study of the attack of the OH and NO radicals to the protein backbone

Name of the conference: Electronic Structure: Principles and applications ESPA 2012

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - poster

City of event: Barcelona, Catalonia, Spain

Date of event: 04/12/2011

End date: 09/12/2011

Organising entity: Universitat Autònoma de

Barcelona

Jon M. Matxain.

Type of entity: University

16 Title of the work: Simulating materials. Quantum and atomistic scale simulations

Name of the conference: 9th Triennial congress of the World Association of Theoretical and Computational Chemists. WATOC 2011

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - others

City of event: Santiago de Compostela, Galicia, Spain

Date of event: 17/07/2011

End date: 22/07/2011

Organising entity: Asociación Mundial de Químicos Teóricos y Computacionales (WATOC)

Jon M. Matxain.

Type of entity: Associations and Groups



- 17** **Title of the work:** Simulating materials. Quantum and atomistic scale simulations
Name of the conference: Second international workshop on multiphysics, multiscale and optimization problems
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Leioa, Spain
Date of event: 06/06/2011
End date: 07/06/2011
Organising entity: Universidad del País Vasco **Type of entity:** University
Jon M. Matxain.
- 18** **Title of the work:** Symmetric assembling modes of polyhedral building blocks
Name of the conference: Symmetry Conference (ISIS 2010)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Gmuend, Austria
Date of event: 23/08/2010
End date: 28/08/2010
Organising entity: ISIS Symmetry **Type of entity:** Associations and Groups
Jon M. Matxain.
- 19** **Title of the work:** Endohedral compounds of hollow ZnS nanostructures
Name of the conference: Electronic Structure: Principles and Applications (ESPA) 2010
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - poster
City of event: Oviedo, Principality of Asturias, Spain
Date of event: 29/06/2010
End date: 03/07/2010
Organising entity: Universidad de Oviedo **Type of entity:** University
Jon M. Matxain.
- 20** **Title of the work:** Endohedral compounds of Hollow ZnS nanostructures
Name of the conference: ICCMSE Conference
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Rodas, Greece
Date of event: 09/2009
Organising entity: Universidad de Atenas **Type of entity:** University
Jon M. Matxain.
- 21** **Title of the work:** ZnS nanoclusters in biological environment
Name of the conference: Theoretical Biophysics 2009 (Theobio 09)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Roscoff, France
Date of event: 06/2009
Organising entity: Universidad de Paris **Type of entity:** University
Jon M. Matxain.



- 22** **Title of the work:** Thermally stable solids based on endohedrally doped ZnS nanoclusters
Name of the conference: Molecular Informatics and Bioinformatics (MolInfBioInf 09)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Budapest, Hungary
Date of event: 03/2009
Organising entity: Universidad de Budapest **Type of entity:** University
Jon M. Matxain.
- 23** **Title of the work:** Magnetic endohedral transition metal doped semiconducting nanoclusters
Name of the conference: 19 Conferencia de Química
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Santiago de Cuba, Cuba
Date of event: 12/2008
Organising entity: Universidad de Oriente **Type of entity:** University
Jon M. Matxain.
- 24** **Title of the work:** Nobel building blocks for Molecular solids and Spintronics?
Name of the conference: Electronic Structure: Principles and Applications (ESPA) 2008
Type of event: Conference **Geographical area:** Internacional
Type of participation: 'Participatory - poster
City of event: Palma de Mallorca, Balearic Islands, Spain
Date of event: 09/2008
Organising entity: Universidad de las Islas Baleares **Type of entity:** University
Jon M. Matxain.
- 25** **Title of the work:** Magnetic endohedral transition metal doped semiconducting nanoclusters
Name of the conference: Molecular Informatics and Bioinformatics (MolInfBioInf 08)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Budapest, Hungary
Date of event: 03/2008
Organising entity: Universidad de Budapest **Type of entity:** University
Jon M. Matxain.
- 26** **Title of the work:** Mn@Sn₁₂ stannaspherene dimer. Ferromagnetic or Antiferromagnetic?
Name of the conference: Trends in Nanotechnology 2007 (TNT 07)
Type of event: Conference **Geographical area:** Internacional
Type of participation: 'Participatory - poster
City of event: Donostia, Spain
Date of event: 09/2007
Organising entity: Donostia International Physics Center **Type of entity:** Centro de Investigación
Jon M. Matxain.
- 27** **Title of the work:** Antioxidant properties of pyridoxine
Name of the conference: Theoretical Biophysics 2007 (Theobio 07)
Type of event: Conference **Geographical area:** Internacional
Type of participation: Participatory - invited/keynote talk
City of event: Cetraro, Italy



Date of event: 06/2007

Organising entity: Universidad de Calabria
Jon M. Matxain.

Type of entity: University

28 Title of the work: Structure and optical properties of ZnS nanoclusters

Name of the conference: ASEVA workshop 19

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - oral communication

City of event: Avila, Castile and León, Spain

Date of event: 09/2006

Organising entity: Asociacion española del vacio
ASEVA

Type of entity: Associations and Groups

Jon M. Matxain.

29 Title of the work: Theoretical study of the antioxidant properties of pyridoxine

Name of the conference: Electronic Structure: Principles and Applications (ESPA) 2006

Type of event: Conference

Geographical area: Internacional

Type of participation: 'Participatory - poster

City of event: Santiago de Compostela, Galicia, Spain

Date of event: 07/2006

Organising entity: Universidad de Santiago de
Compostela

Type of entity: University

Jon M. Matxain.

30 Title of the work: Electronic excitation energies of ZnS nanoparticles

Name of the conference: Nanospain 2006

Type of event: Conference

Geographical area: Internacional

Type of participation: 'Participatory - poster

City of event: Pamplona, Spain

Date of event: 03/2006

Organising entity: Nanospain

City organizing entity: Spain

Jon M. Matxain.

31 Title of the work: Diffusion Monte Carlo applied to photochemical problems

Name of the conference: Theoretical Biophysics 2005 (THEOBIO 05)

Type of event: Conference

Geographical area: Internacional

Type of participation: Participatory - invited/keynote talk

City of event: Örebro, Sweden

Date of event: 29/06/2005

End date: 02/07/2005

Organising entity: University of Örebro

Type of entity: University

City organizing entity: örebro, Sweden

Jon M. Matxain.

32 Title of the work: Discordant results on the $\text{FeO}^+ + \text{H}_2$ reaction reconciled by Quantum Monte Carlo theory

Name of the conference: Electronic Structure: Principles and Applications (ESPA) 2004

Type of event: Conference

Geographical area: Internacional

Type of participation: 'Participatory - poster

City of event: Valladolid, Castile and León, Spain

Date of event: 09/2004



Organising entity: Universidad de Valladolid
Jon M. Matxain.

Type of entity: University

33 Title of the work: Equipo organizador

Name of the conference: Theoretical Biophysics 2003 (THEOBIO 03)

Type of event: Conference

Geographical area: Internacional

Type of participation: Organizational -Others

City of event: Donostia, Basque Country, Spain

Date of event: 03/2003

Organising entity: Universidad del País Vasco
Jon M. Matxain.

Type of entity: University

34 Title of the work: Small clusters of II-VI materials

Name of the conference: Electronic Structure: Principles and Applications (ESPA) 2002

Type of event: Conference

Geographical area: Internacional

Type of participation: 'Participatory - poster

City of event: Sevilla, Andalusia, Spain

Date of event: 09/2002

Organising entity: Universidad de Sevilla
Jon M. Matxain.

Type of entity: University

35 Title of the work: Equipo organizador

Name of the conference: One-day workshop on Physical Chemistry

Type of event: Conference

Geographical area: Internacional

Type of participation: Organizational -Others

City of event: Donostia, Basque Country, Spain

Date of event: 05/07/2001

End date: 05/07/2001

Organising entity: Universidad del País Vasco
Jon M. Matxain.

Type of entity: University

36 Title of the work: Small clusters of II-VI materials: Zn_iS_j, i=1-9,12,15. Structure characterization and excitation energies

Name of the conference: Electronic Structure: Principles and Applications (ESPA) 2000

Type of event: Conference

Geographical area: Internacional

Type of participation: 'Participatory - poster

City of event: Donostia, Basque Country, Spain

Date of event: 10/2000

Organising entity: Universidad del País Vasco
Jon M. Matxain.

Type of entity: University

37 Title of the work: Equipo organizador

Name of the conference: International conference on electron densities and electron distributions

Type of event: Conference

Geographical area: Internacional

Type of participation: Organizational -Others

City of event: Donostia, Basque Country, Spain

Date of event: 04/2000

Organising entity: Universidad del País Vasco
Jon M. Matxain.

Type of entity: University

- 38** **Title of the work:** Equipo organizador
Name of the conference: International Workshop on Electronic Structure: Prediction and Applications II
Type of event: Conference **Geographical area:** Internacional
Type of participation: Organizational -Others
City of event: Donostia, Basque Country, Spain
Date of event: 06/1999
Organising entity: Universidad del País Vasco **Type of entity:** University
Jon M. Matxain.
- 39** **Title of the work:** How strong are hydrogen bonds in benzoquinone crystals?
Name of the conference: Undergraduate research in chemistry. PAC symposium '98
Type of event: Conference **Geographical area:** Holanda
Type of participation: 'Participatory - poster
City of event: Leiden, Holland
Date of event: 03/1998
Organising entity: PAC **Type of entity:** Associations and Groups
City organizing entity: Amsterdam, Holland
Jon M. Matxain.
- 40** **Title of the work:** How strong are hydrogen bonds in benzoquinone crystals?
Name of the conference: Stichting Scheikundig Onderzoek in Nederland (SON), Werkgemeenschap voor spectroscopie en theorie
Type of event: Conference **Geographical area:** Holanda
Type of participation: 'Participatory - poster
City of event: Lunteren, Holland
Date of event: 02/1998
Organising entity: The Royal Netherlands Chemical Society **Type of entity:** Associations and Groups
City organizing entity: Amsterdam, Holland

R&D management and participation in scientific committees

Organization of R&D activities

- 1** **Title of the activity:** Euskal Esperientziak Zientzia Zabalkuntzan
Type of activity: Workshop **Geographical area:** Regional
City of event: Donostia, Basque Country, Spain
Convening entity: Universidad del País Vasco **Type of entity:** University
City convening entity: Donostia, Basque Country, Spain
Type of participation: Organiser
Start-End date: 14/06/2018 - 15/06/2018 **Duration:** 2 days
- 2** **Title of the activity:** iPolymorphs
Type of activity: Workshop **Geographical area:** Mundial
City of event: Donostia, Basque Country, Spain
Convening entity: Universidad del País Vasco **Type of entity:** University
City convening entity: Donostia, Basque Country, Spain
Type of participation: Organiser
Start-End date: 22/06/2016 - 24/06/2016 **Duration:** 3 days



- 3** **Title of the activity:** Computation of Electronic Excited States
Type of activity: Summer School **Geographical area:** Mundial
City of event: Donostia, Basque Country, Spain
Convening entity: Universidad del País Vasco **Type of entity:** University
City convening entity: Donostia, Basque Country, Spain
Type of participation: Organiser
Start-End date: 01/09/2015 - 04/09/2015 **Duration:** 4 days
- 4** **Title of the activity:** International conference on Electron densities and electron distributions
Type of activity: Congreso Internacional **Geographical area:** Mundial
City of event: Donostia, Basque Country, Spain
Convening entity: Universidad del País Vasco **Type of entity:** University
City convening entity: Donostia, Basque Country, Spain
Type of participation: Co-organizador
Start-End date: 01/04/2000 - 04/04/2000 **Duration:** 3 days
- 5** **Title of the activity:** International Workshop on Electronic Structure: Predictions and Applications II
Type of activity: Workshop **Geographical area:** Mundial
City of event: Donostia, Basque Country, Spain
Convening entity: Universidad del País Vasco **Type of entity:** University
City convening entity: Donostia, Basque Country, Spain
Type of participation: Co-organizador
Start date: 06/1999 **Duration:** 1 day

Other achievements

Stays in public or private R&D centres

- 1** **Entity:** Universitat de Girona **Type of entity:** University
Faculty, institute or centre: Instituto Universitario de Química Computacional
City of entity: Girona, Holland
Primary (UNESCO code): 230226 - Physical biochemistry
Start-End date: 16/01/2013 - 20/01/2013 **Duration:** 5 days
Goals of the stay: Guest
- 2** **Entity:** Universidad de Örebro **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias Naturales
City of entity: Örebro, Sweden
Primary (UNESCO code): 230226 - Physical biochemistry
Start-End date: 01/01/2005 - 31/12/2006 **Duration:** 2 years
Goals of the stay: Post-doctoral
- 3** **Entity:** Universidad de Cambridge
Faculty, institute or centre: Cavendish Laboratory
City of entity: Utrecht, Holland
Primary (UNESCO code): 230226 - Physical biochemistry
Start-End date: 01/07/2001 - 30/09/2001 **Duration:** 3 months
Goals of the stay: Estancia Predoctoral



- 4** **Entity:** Universidad Jaime I **Type of entity:** University
City of entity: Castellon, Valencian Community, Spain
Primary (UNESCO code): 230226 - Physical biochemistry
Start-End date: 24/01/2000 - 22/02/2000 **Duration:** 1 month
Goals of the stay: Estudiante
- 5** **Entity:** Universidad de Utrecht
Faculty, institute or centre: Facultad de Química
City of entity: Utrecht, Holland
Primary (UNESCO code): 230226 - Physical biochemistry
Start-End date: 01/09/1996 - 30/06/1998 **Duration:** 1 year - 10 months
Goals of the stay: Estudiante

Obtained grants and scholarships

- 1** **Name of the grant:** Ayuda a la realización de cursos de doctorado en otra universidad
Aims: Pre-doctoral
Awarding entity: MINISTERIO DE EDUCACION Y CIENCIA
Conferral date: 01/01/2000 **Duration:** 1 month
Entity where activity was carried out: Universidad Jaime I
- 2** **Name of the grant:** Beca Predoctoral
Aims: Pre-doctoral
Awarding entity: Universidad del País Vasco **Type of entity:** University
Conferral date: 01/10/1998 **Duration:** 4 years
Entity where activity was carried out: Universidad del País Vasco
Faculty, institute or centre: Facultad de Ciencias Químicas
- 3** **Name of the grant:** Beca Erasmus
Aims: Erasmus
Awarding entity: Union Europea **Type of entity:** publico
Conferral date: 01/09/1996 **Duration:** 1 year
Entity where activity was carried out: Universidad de Utrecht
Faculty, institute or centre: Facultad de Química

Prizes, mentions and distinctions

- 1** **Description:** Premio Especial Martin Guzmán
Awarding entity: Rotary Club **Type of entity:** Associations and Groups
City awarding entity: Donostia, Basque Country, Spain
Conferral date: 2004
- 2** **Description:** Premio Extraordinario de Doctorado
Awarding entity: Universidad del País Vasco **Type of entity:** University
Conferral date: 2003



Obtained accreditations/recognitions

- 1** **Description:** Evaluación positiva Acreditación I3
Accrediting entity: Agencia Nacional de Evaluación y Prospectiva
Date of recognition: 18/01/2013
- 2** **Description:** Evaluación positiva Personal Doctor Investigador
Accrediting entity: UNIBASQ
Date of recognition: 09/10/2012
- 3** **Description:** Evaluación positiva Profesor Adjunto
Accrediting entity: UNIBASQ
Date of recognition: 09/10/2012
- 4** **Description:** Evaluación positiva Profesor Agregado
Accrediting entity: UNIBASQ
Date of recognition: 09/10/2012
- 5** **Description:** Evaluación positiva Profesor Ayudante Doctor
Accrediting entity: Agencia Nacional de Evaluación de la Calidad y Acreditación
Date of recognition: 13/04/2004