



Eva Maria Fernandez Sanchez

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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.

I graduated in Physics at the Universidad de Valladolid in 2001. Then I started my research career with a FPU grant from the Spanish Ministry of Science to work on the PhD at the department of “Física Teórica, Atómica y Óptica” at the Universidad de Valladolid supervised by Prof. Luis C. Balbás. In December 2005 I obtained the PhD degree with the highest marks. My PhD was awarded Special Doctorate Award by the Universidad de Valladolid in the year 2007. From March 2006 to March 2008 I joined as postdoc at the Technical University of Denmark for two years. From March 2008 to October 2018 I worked as research at the Instituto de Ciencia de Materiales de Madrid (ICMM) of the Consejo Superior de Investigaciones Científicas (CSIC), firstly with a JaeDoc Postdoctoral contract and then with a Comunidad de Madrid postdoctoral contract associated to project. From November 2012 I develop my research work at the department of Física Fundamental of the Universidad Nacional de Educación a Distancia, initially with a competitive postdoctoral contract of the UNED and from November 2015 with a Ramón y Cajal contract.

I have published 38 papers (one Angew. Chem. Int., one Physical Review Letters and seven Physical Review B) with have received more than 1390 citations altogether. Twelve of my papers have received more than 25 citations (one of them has received more than 415 citations) and my Hirsch index is $h=16$. I have participated in 11 research project, one international project funding by the Danish Research Agency and 6 national projects (one of them in collaboration with Osnabrück University, Germany).

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

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

I work in two research lines:

1. Nanometric cluster

Improvement and proposal of catalysts for the adsorption of H₂, O₂, CO and CO oxidation on doped clusters. The main interest is the search for new catalysts more active for the oxidation of CO and more efficient materials for hydrogen storage. The analysis of the role played by the dopant atom in the reactivity of these aggregates according to their size and composition allows to improve or design new more efficient catalysts for the oxidation of CO (avoiding or reducing their emission to the atmosphere since when inhaled in high levels can cause death in a few minutes) or for hydrogen storage (the main difficulty for the use of hydrogen as an energy source is its storage in a safe, reliable and compact way).

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

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

**Eva Maria Fernandez Sanchez**

Surname(s): **Fernandez Sanchez**
 Name: **Eva Maria**
 DNI: **44906568B**
 Date of birth: **13/11/1978**
 Gender: **Female**
 Nationality: **Spain**
 Country of birth: **Spain**
 Aut. region/reg. of birth: **Castile and León**
 Contact province: **Madrid**
 City of birth: **Valladolid**
 Contact address: **Paseo Senda del Rey**
 Rest of contact address: **9**
 Postcode: **28040**
 Contact country: **Spain**
 Contact aut. region/reg.: **Community of Madrid**
 Contact city: **Madrid**
 Land line phone: **913988863**
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 Personal web page: **http://portal.uned.es/portal/page?_pageid=93,25912601&_dad=portal&_schema=PORTAL**

Current professional situation

Employing entity: Universidad Nacional de Educación a Distancia **Type of entity:** University
Department: Física Fundamental, Facultad de Ciencias
Professional category: Investigadora Ramón y Cajal
Start date: 01/11/2015
Type of contract: PDI Contrato Postdoc **Dedication regime:** Full time
Primary (UNESCO code): 221001 - Catalysis; 221016 - Interfacial chemistry; 221018 - Liquid state physics; 221100 - Solid state physics
Secondary (UNESCO code): 221018 - Liquid state physics

Previous positions and activities

	Employing entity	Professional category	Start date
1	Universidad Nacional de Educación a Distancia	PDI postdoc	01/11/2012
2	Instituto de Ciencia de Materiales de Madrid	Postdoc CAM	01/01/2011
3	Instituto de Ciencia de Materiales de Madrid	Postdoc JaeDoc	16/03/2008
4	Technical University of Denmark	Postdoc	01/03/2006



	Employing entity	Professional category	Start date
5	Universidad de Valladolid	Becario FPU	01/01/2002

- 1** **Employing entity:** Universidad Nacional de Educación a Distancia
Professional category: PDI postdoc
Start-End date: 01/11/2012 - 31/10/2015

Type of entity: University
Duration: 3 years
- 2** **Employing entity:** Instituto de Ciencia de Materiales de Madrid
Professional category: Postdoc CAM
Start-End date: 01/01/2011 - 31/10/2012

Type of entity: State agency
Duration: 1 year - 10 months
- 3** **Employing entity:** Instituto de Ciencia de Materiales de Madrid
Professional category: Postdoc JaeDoc
Start-End date: 16/03/2008 - 31/12/2010

Type of entity: State agency
Duration: 2 years - 9 months - 15 days
- 4** **Employing entity:** Technical University of Denmark
Professional category: Postdoc
Start-End date: 01/03/2006 - 29/02/2008

Type of entity: University
Duration: 2 years
- 5** **Employing entity:** Universidad de Valladolid
Professional category: Becario FPU
Start-End date: 01/01/2002 - 31/12/2005

Type of entity: University
Duration: 4 years



Education

University education

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

- 1 University degree:** DEA
Name of qualification: Diploma de Estudios Avanzados
Degree awarding entity: Universidad de Valladolid **Type of entity:** University
Date of qualification: 30/06/2003
- 2 University degree:** Higher degree
Name of qualification: Licenciado en Física
Degree awarding entity: Universidad de Valladolid **Type of entity:** University
Date of qualification: 2001

Doctorates

Doctorate programme: Programa Oficial de Doctorado en Física
Degree awarding entity: Universidad de Valladolid **Type of entity:** University
Date of degree: 16/12/2005
DEA awarding entity: Universidad de Valladolid
Date DEA was awarded: 2003
Thesis title: Reactividad frente a O₂ y CO de agregados nanométricos de oro libres y soportados sobre alúmina. Estudio a partir de primeros principios.
Thesis director: Luis Carlos Balbás
Obtained qualification: Sobresaliente Cum laude
Special doctorate award: Yes **Date of award:** 2007

Attended advanced, improvement and innovative teacher training and new technology courses and seminars focused on improving teaching

Title of course/seminar: Certificado de Aptitud Pedagógica (CAP)
Organising entity: Universidad Complutense de Madrid **Type of entity:** University
Faculty, institute or centre: Facultad de Educación
Duration in hours: 60 hours
Start-End date: 01/10/2001 - 30/06/2002



Language skills

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

Teaching experience

General teaching experience

- 1 Type of teaching:** Official teaching
Name of the course: Mecánica Cuántica
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Grado en Física
Course given: Primero **Frequency of the activity:** 1
Start date: 2018 **End date:** 2019
End date: 2019 **Type of hours/ ECTS credits:** Credits
Hours/ECTS credits: 6
Entity: Universidad Nacional de Educación a Distancia **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 2 Name of the course:** Modelización y Simulación de Sistemas Complejos
University degree: Master en Física de Sistemas Complejos
Start date: 2016 **End date:** 2019
End date: 2019
Entity: Universidad Nacional de Educación a Distancia **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 3 Type of teaching:** Official teaching
Name of the course: Física Cuántica II
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Grado en Física
Course given: tercero **Frequency of the activity:** 1
Start date: 2014 **End date:** 2019
End date: 2019 **Type of hours/ ECTS credits:** Credits
Hours/ECTS credits: 6
Entity: Universidad Nacional de Educación a Distancia **Type of entity:** University
Faculty, institute or centre: Facultad de Ciencias
- 4 Type of teaching:** Official teaching
Name of the course: Fundamentos de Física I
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Grado en Física



Course given: Primero
Start date: 2014
End date: 2016
Hours/ECTS credits: 6
Entity: Universidad Nacional de Educación a Distancia
Faculty, institute or centre: Facultad de Ciencias

Frequency of the activity: 1
End date: 2016
Type of hours/ ECTS credits: Credits
Type of entity: University

5 **Type of teaching:** Official teaching
Name of the course: Física Cuántica
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Licenciado en Ciencias Físicas
Frequency of the activity: 1
Start date: 2013
End date: 2014
Hours/ECTS credits: 12
Entity: Universidad Nacional de Educación a Distancia
Faculty, institute or centre: Facultad de Ciencias

End date: 2014
Type of hours/ ECTS credits: Credits
Type of entity: University

6 **Type of teaching:** Official teaching
Name of the course: Mecánica
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Licenciado en Ciencias Químicas
Frequency of the activity: 1
Start date: 2013
End date: 2013
Hours/ECTS credits: 12
Entity: Universidad Nacional de Educación a Distancia
Faculty, institute or centre: Facultad de Ciencias

End date: 2013
Type of hours/ ECTS credits: Credits
Type of entity: University

7 **Type of teaching:** Official teaching
Name of the course: Mecánica Cuántica
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Licenciado en Ciencias Físicas
Frequency of the activity: 1
Start date: 2013
End date: 2013
Hours/ECTS credits: 6
Entity: Universidad Nacional de Educación a Distancia
Faculty, institute or centre: Facultad de Ciencias

End date: 2013
Type of hours/ ECTS credits: Credits
Type of entity: University

8 **Type of teaching:** Official teaching
Name of the course: Física
Type of programme: Bachelor's degree
Type of subject: Obligatory
University degree: Grado en Química
Course given: Primero
Start date: 2012
End date: 2012

Type of teaching: Laboratory work
Frequency of the activity: 1
End date: 2013
Type of hours/ ECTS credits: Credits



Hours/ECTS credits: 2,1

Entity: Universidad Autónoma de Madrid

Faculty, institute or centre: Facultad de Ciencias

Type of entity: University

9 Type of teaching: Official teaching

Name of the course: Física

Type of programme: Bachelor's degree

Type of subject: Obligatory

University degree: Grado en Biología

Course given: Primero

Start date: 2010

End date: 2011

Hours/ECTS credits: 3,6

Entity: Universidad Autónoma de Madrid

Faculty, institute or centre: Facultad de Ciencias

Type of teaching: Laboratory work

Frequency of the activity: 1

End date: 2011

Type of hours/ ECTS credits: Credits

Type of entity: University

10 Type of teaching: Official teaching

Name of the course: Física

Type of programme: Bachelor's degree

Type of subject: Obligatory

University degree: Grado en Ciencias Ambientales

Course given: Segundo

Start date: 2009

End date: 2010

Hours/ECTS credits: 3,2

Entity: Universidad Autónoma de Madrid

Faculty, institute or centre: Facultad de Ciencias

Type of teaching: Laboratory work

Frequency of the activity: 1

End date: 2010

Type of hours/ ECTS credits: Credits

Type of entity: University

11 Type of teaching: Official teaching

Name of the course: Física Atómica y Molecular

Type of programme: Bachelor's degree

Type of subject: Optional

University degree: licenciado en Física

Course given: Quinto

Start date: 2003

End date: 2005

Hours/ECTS credits: 1

Entity: Universidad de Valladolid

Faculty, institute or centre: Facultad de Ciencias

Department: Física Teórica Atómica y Óptica

Type of teaching: In person theory

Frequency of the activity: 2

End date: 2005

Type of hours/ ECTS credits: Credits

Type of entity: University

12 Type of teaching: Official teaching

Name of the course: Técnicas Experimentales en Física Cuántica

Type of programme: Bachelor's degree

Type of subject: Obligatory

University degree: licenciado en Física

Course given: tercer

Start date: 2003

End date: 2004

Hours/ECTS credits: 8

Entity: Universidad de Valladolid

Type of teaching: Laboratory work

Frequency of the activity: 1

End date: 2004

Type of hours/ ECTS credits: Credits

Type of entity: University



Faculty, institute or centre: Facultad de Ciencias
Department: Física Teórica Atómica y Óptica

Experience supervising doctoral thesis and/or final year projects

- Project title:** TFM: Estudio de la estructura del estado fundamental y la adsorción de O₂ de agregados nanométricos de oro dopados con vanadio AunVm.
Entity: Universidad Nacional de Educación a Distancia **Type of entity:** University
Student: Sergio Garcia Gonzalez
Date of reading: 11/03/2016
- Project title:** TFM: Estudio de las Ondas Electromagnéticas para Bachillerato y Acceso a la Universidad
Entity: Universidad Nacional de Educación a Distancia **Type of entity:** University
Student: Concepción García
Date of reading: 2015

Scientific and technological experience

Scientific or technological activities

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

- Name of the project:** Contrato Predoctoral garantía juvenil Comunidad de Madrid 1 año.
Entity where project took place: Universidad Nacional de Educación a Distancia **Type of entity:** University
Nº of researchers: 1
Start-End date: 07/03/2018 - 06/03/2019
- Name of the project:** premio "L'Oreal-UNESCO for Women in Science en España"
Entity where project took place: L'Oreal
Nº of researchers: 1
Start-End date: 01/01/2018 - 31/12/2018
Total amount: 15.000 €
- Name of the project:** Estructura, dinámica y propiedades electrónicas de nanoagregados atómicos, nanoaleaciones, interfases y líquidos metálicos de interés tecnológico en espintrónica, catálisis y reactores nucleares.
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Universidad de Valladolid **Type of entity:** University
City of entity: Valladolid, Castile and León, Spain
Name principal investigator (PI, Co-PI....): A. Aguado
Funding entity or bodies:
Junta de Castilla y León **Type of entity:** Public Administration
City funding entity: Valladolid, Castile and León, Spain



Name of the programme: Apoyo a proyectos de investigación de la Junta de Castilla y León
Start-End date: 01/01/2011 - 31/12/2013 **Duration:** 2 years

- 4** **Name of the project:** Structure and Dynamic of complex fluids and their interface.
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Instituto de Ciencia de Materiales de Madrid **Type of entity:** State agency
City of entity: Madrid, Community of Madrid, Spain
Name principal investigator (PI, Co-PI....): E. Chacón
Funding entity or bodies: Ministerio de Ciencia e Innovación. Investigación **Type of entity:** Public Administration
City funding entity: Madrid, Community of Madrid, Spain
Start-End date: 01/01/2011 - 31/12/2013
Dedication regime: Part time
- 5** **Name of the project:** Modelling and simulation of Complex Systems.
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** Regional
Degree of contribution: Researcher
Entity where project took place: Instituto de Ciencia de Materiales de Madrid **Type of entity:** State agency
Name principal investigator (PI, Co-PI....): E. Chacón
Funding entity or bodies: Comunidad de Madrid **Type of entity:** Public Administration
City funding entity: Madrid, Community of Madrid, Spain
Start-End date: 01/01/2010 - 31/12/2013
Dedication regime: Full time
- 6** **Name of the project:** Electronic and morphological properties of nanostructured materials of interest in spintronics, catalysis and new alloys.
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: Universidad de Valladolid **Type of entity:** University
Name principal investigator (PI, Co-PI....): A. Vega
Funding entity or bodies: Ministerio de Ciencia e Innovación **Type of entity:** Public Administration
City funding entity: Madrid, Community of Madrid, Spain
Start-End date: 01/01/2009 - 31/12/2011
Dedication regime: Part time
- 7** **Name of the project:** Structure and Dynamic of complex fluids and their interface.
Type of project: Basic research (including archaeological digs, etc)
Degree of contribution: Researcher
Entity where project took place: Instituto de Ciencia de Materiales de Madrid **Type of entity:** State agency
Name principal investigator (PI, Co-PI....): E. Chacón

**Funding entity or bodies:**Ministerio de Ciencia e Innovación. Investigación **Type of entity:** Public Administration**City funding entity:** Madrid, Community of Madrid, Spain**Start-End date:** 01/01/2008 - 31/12/2009**Dedication regime:** Part time**8 Name of the project:** New electrode materials for hydrogen evolution.**Geographical area:** National**Degree of contribution:** Researcher**Entity where project took place:** Technical University of Denmark**Type of entity:** University**City of entity:** Denmark**Funding entity or bodies:**

Danish Research Agency, Ministry of Science Technology and Innovation, Denmark.

Type of entity: Public Research Body**Start-End date:** 01/01/2005 - 31/12/2007**Dedication regime:** Full time**9 Name of the project:** Theoretical study of the structural, electronic, and thermal properties of nanometric systems of technological interest**Type of project:** Basic research (including archaeological digs, etc)**Geographical area:** National**Entity where project took place:** Universidad de Valladolid**Name principal investigator (PI, Co-PI....):** A. Vega**Funding entity or bodies:**

Ministry of Science, and Technology

Type of entity: Public Administration**Start-End date:** 01/01/2005 - 01/01/2007**Dedication regime:** Full time**10 Name of the project:** Reactivity of nanometric clusters**Type of project:** Basic research (including archaeological digs, etc)**Geographical area:** European Union**Degree of contribution:** Researcher**Entity where project took place:** Valladolid University and Osnabruck University**Name principal investigator (PI, Co-PI....):** L. C. Balbás; G. Borstel**Funding entity or bodies:**

MINISTERIO DE EDUCACION Y CIENCIA

City funding entity: Spain**Name of the programme:** Acciones Integradas**Start-End date:** 01/01/2004 - 31/12/2005**Dedication regime:** Full time**11 Name of the project:** Modelling of electronic-molecular nanostructures and metallic compounds (Modelización electrónico-molecular de nanoestructuras)**Type of project:** Basic research (including archaeological digs, etc)**Geographical area:** National**Degree of contribution:** Researcher**Entity where project took place:** Universidad de Valladolid**Type of entity:** University**City of entity:** Valladolid, Castile and León, Spain



Name principal investigator (PI, Co-PI....): Dr. P. Iñiguez

Funding entity or bodies:

Ministry of Science, and Technology

Type of entity: Public Research Body

Start-End date: 01/01/2003 - 31/12/2005

Dedication regime: Full time

12 Name of the project: Electronic, structural and thermal properties of nanometric metals and metal oxides: study and simulation from first principles.

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

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): L. C. Balbás

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Public Administration

City funding entity: Valladolid, Castile and León, Spain

Start-End date: 01/01/2003 - 31/12/2004

Dedication regime: Full time

13 Name of the project: Study of new nanometric materials.

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

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Universidad de Valladolid

Type of entity: University

City of entity: Valladolid, Castile and León, Spain

Name principal investigator (PI, Co-PI....): L. C. Balbás

Funding entity or bodies:

Junta de Castilla y León

Type of entity: Public Administration

City funding entity: Valladolid, Castile and León, Spain

Start-End date: 01/01/2002 - 31/12/2004

Dedication regime: Full time



Scientific and technological activities

Scientific production

Publications, scientific and technical documents

- 1** Maiye Jia; Jan Vanbuel; Pierro Ferrari; Eva M. Fernández; Sandy Gewinner; Wieland Schöllkopf; Minh Tho NGuyen; André Fieclicke; Ewald Janssens. Size Dependent H₂ Adsorption on AlnRh⁺ (n = 1–12) Clusters. Chemistry-a European Journal. 23, pp. 15638 - 15643. 2018.

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

Corresponding author: No

Impact source: ISI **Category:** MATERIALS SCIENCE, MULTIDISCIPLINARY

Impact index in year of publication: 4.484 **Journal in the top 25%:** Yes

Position of publication: 54 **No. of journals in the cat.:** 285

Relevant publication: Yes
- 2** Jan Vanbuel; Eva M. Fernández; Pierro Ferrari; Sandy Gewinner; Wieland Schöllkopf; L. Carlos Balbás; André Fieclicke; Ewald Janssens. Hydrogen Chemisorption on Singly Vanadium-Doped Aluminum Clusters. Chemistry-a European Journal. 23, pp. 15638 - 15643. 2017.

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

Corresponding author: No

Impact source: ISI **Category:** CHEMISTRY, MULTIDISCIPLINARY

Impact index in year of publication: 5.16 **Journal in the top 25%:** Yes

Position of publication: 37 **No. of journals in the cat.:** 171

Relevant publication: Yes
- 3** EM Fernandez; E Chacon; P Tarazona; AO Parry; C Rascon. Intrinsic Fluid Interfaces and Nonlocality. Phys. Rev. Lett. 111, pp. 096104 - 096104. American Physical Society, 08/2013. Available on-line at: <<http://link.aps.org/doi/10.1103/PhysRevLett.111.096104>>.

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

Impact source: ISI **Category:** Science Edition - PHYSICS, MULTIDISCIPLINARY

Impact index in year of publication: 7.943 **Journal in the top 25%:** Yes

Position of publication: 5 **No. of journals in the cat.:** 83

Source of citations: WOS **Citations:** 17

Relevant publication: Yes
- 4** S Wang; V Petzold; V Tripkovic; J Kleis; JG Howalt; E Skulason; EM Fernandez; B Hvolbaek; G Jones; A Toftelund; H Falsig; M Bjorketun; F Studt; F Abild-Pedersen; J Rossmeisl; JK Norskov; T Bligaard. Universal transition state scaling relations for (de)hydrogenation over transition metals. Physical Chemistry Chemical Physics. 13 - 46, pp. 20760 - 20765. 2011.

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

Impact source: ISI **Category:** Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Impact index in year of publication: 3.573 **Journal in the top 25%:** Yes



Position of publication: 5

Source of citations: WOS

Relevant publication: Yes

No. of journals in the cat.: 33

Citations: 141

- 5** EM Fernandez; PG Moses; A Toftelund; et al. Scaling relationships for adsorption energies on transition metal oxide, sulfide, and nitride surfaces. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION. 47 - 25, pp. 4683 - 4686. 2008.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 10.879

Position of publication: 4

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: Science Edition - CHEMISTRY, MULTIDISCIPLINARY

Journal in the top 25%: Yes

No. of journals in the cat.: 127

Citations: 131

- 6** MB Torres; EM Fernandez; LC Balbas. Theoretical study of isoelectronic SinM clusters ($M=\text{Sc}, \text{Ti}, \text{V}^+$; $n=14-18$). PHYSICAL REVIEW B. 75 - 20, pp. 205425. 2007.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 3.172

Position of publication: 9

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: PHYSICS, CONDENSED MATTER

Journal in the top 25%: Yes

No. of journals in the cat.: 61

Citations: 66

- 7** EM Fernandez; JM Soler; LC Balbas. Planar and cage-like structures of gold clusters: Density-functional pseudopotential calculations. PHYSICAL REVIEW B. 73 - 23, pp. 235433. 2006.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 3.107

Position of publication: 10

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: Science Edition - PHYSICS, CONDENSED MATTER

Journal in the top 25%: Yes

No. of journals in the cat.: 58

Citations: 95

- 8** EM Fernandez; LC Balbas. Theoretical study of CO adsorption on gold/alumina substrates. JOURNAL OF PHYSICAL CHEMISTRY B. 110 - 21, pp. 10449 - 10454. 2006.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 4.115

Position of publication: 17

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: Science Edition - CHEMISTRY, PHYSICAL

Journal in the top 25%: Yes

No. of journals in the cat.: 108

Citations: 11

- 9** EM Fernandez; P Ordejon; LC Balbas. Theoretical study of O-2 and CO adsorption on Au-n clusters ($n=5-10$). CHEMICAL PHYSICS LETTERS. 408 - 4-6, pp. 252 - 257. 2005.

Type of production: Scientific paper

Format: Journal



Impact source: ISI

Impact index in year of publication: 2.438

Position of publication: 8

Source of citations: WOS

Relevant publication: Yes

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

Journal in the top 25%: No

No. of journals in the cat.: 31

Citations: 79

- 10** MB Torres; EM Fernandez; LC Balbas. Theoretical study of structural, electronic, and magnetic properties of $AunM+$ clusters ($M=Sc, Ti, V, Cr, Mn, Fe, Au; n \leq 9$). PHYSICAL REVIEW B. 71 - 15, pp. 155412. 2005.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 3.185

Position of publication: 7

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: Science Edition - PHYSICS, CONDENSED MATTER

Journal in the top 25%: Yes

No. of journals in the cat.: 74

Citations: 99

- 11** EM Fernandez; JM Soler; IL Garzon; LC Balbas. Trends in the structure and bonding of noble metal clusters. PHYSICAL REVIEW B. 70 - 16, pp. 165303. 2004.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 3.075

Position of publication: 8

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: Science Edition - PHYSICS, CONDENSED MATTER

Journal in the top 25%: Yes

No. of journals in the cat.: 60

Citations: 418

- 12** EM Fernandez; LC Balbas; G Borstel; JM Soler. First principles calculation of the geometric and electronic structure of $(Al_2O_3)_n(O-x)$ clusters with $n < 15$ and $x=0, 1, 2$. Thin Solid Films. 428 - 1-2, pp. 206 - 210. 2003.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 1.598

Position of publication: 35

Source of citations: WOS

Relevant publication: Yes

Format: Journal

Category: Science Edition - MATERIALS SCIENCE, MULTIDISCIPLINARY

Journal in the top 25%: Yes

No. of journals in the cat.: 177

Citations: 10

- 13** E. M. Fernández; L. C. Balbás. Multiple adsorption of molecular oxygen on small Au/Pd cationic clusters at finite temperature. A van der Waals density functional study. THE JOURNAL OF CHEMICAL PHYSICS. 144, pp. 224308. 2016.

Type of production: Scientific paper

Corresponding author: Yes

Format: Journal

- 14** EM Fernández; E Chacón; LG MacDowell; P Tarazona. Mesoscopic Hamiltonian for the fluctuations of adsorbed Lennard-Jones liquid films. Physical Review E. 91, pp. 062404. 2015.

Type of production: Scientific paper

Position of signature: 2

Total no. authors: 3

Format: Journal



Impact source: ISI

Impact index in year of publication: 2.288

Position of publication: 5

Category: PHYSICS, MATHEMATICAL

Journal in the top 25%: Yes

No. of journals in the cat.: 54

- 15** E Chacon; EM Fernandez; P Tarazona. The effect of dispersion forces on the capillary waves fluctuations of liquid surfaces. Physical Review E. 89, pp. 042406. 2014.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 2.326

Position of publication: 6

Format: Journal

Category: Science Edition - PHYSICS, MATHEMATICAL

Journal in the top 25%: Yes

No. of journals in the cat.: 55

- 16** P. G. Moses; L. C. Grabow; E. M. Fernandez; B. Hinnemann; H. Topsøe; K. G. Knudsen; J. K. Nørskov. Trends in hydrodesulfurization catalysis based on realistic surface models. Catalysis Letters. 144, pp. 1425. 2014.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 2.291

Position of publication: 62

Source of citations: WOS

Format: Journal

Category: CHEMISTRY, PHYSICAL

Journal in the top 25%: No

No. of journals in the cat.: 135

Citations: 24

- 17** EM Fernández; A Vega; LC Balbás. Theoretical study of AlnV+ clusters and their interaction with Ar. Journal of Chemical Physics. 11/2013.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 3.164

Position of publication: 8

Impact source: ISI

Impact index in year of publication: 3.164

Position of publication: 8

Source of citations: WOS

Source of citations: WOS

Category: PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: Yes

No. of journals in the cat.: 34

Category: PHYSICS, ATOMIC, MOLECULAR & CHEMICAL

Journal in the top 25%: Yes

No. of journals in the cat.: 34

Citations: 1

Citations: 4

- 18** H Cantera-López; EM Fernandez; LC Balbas; G. Borstel. Adsorption of H, H₂, and H₂O inside and outside of (M@Si₁₆F)₆ tube-like aggregates and wires (M = V, Ta). A first principles study. Materials Chemistry and Physics. 139, pp. 247 - 255. Sending, 2013.

Type of production: Scientific paper

Impact source: ISI

Impact index in year of publication: 2.234

Position of publication: 51

Source of citations: WOS

Format: Journal

Category: Science Edition - MATERIALS SCIENCE, MULTIDISCIPLINARY

Journal in the top 25%: Yes

No. of journals in the cat.: 232

Citations: 2



- 19** EM Fernandez; E Chacon; P Tarazona. Capillary wave spectrum at adsorbed liquid films. *Physical Review B*. 86 - 8, pp. 085401. 2012.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.691
Position of publication: 13
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, CONDENSED MATTER
Journal in the top 25%: Yes
No. of journals in the cat.: 69
Citations: 10
- 20** EM Fernandez; MB Torres; LC Balbas. First Principles Study of CO Adsorption-CO₂ Desorption Mechanisms on Oxidized Doped-Gold Cationic Clusters MAunOm⁺ (M = Ti, Fe; n=1, 4-7; m=1-2). *International Journal of Quantum Chemistry*. 111 - 2, pp. 510 - 519. 2011.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.357
Position of publication: 25
Source of citations: WOS
Format: Journal
Category: MATHEMATICS, INTERDISCIPLINARY APPLICATIONS
Journal in the top 25%: No
No. of journals in the cat.: 25
Citations: 5
- 21** EM Fernandez; LC Balbas. GGA versus van der Waals density functional results for mixed gold/mercury molecules and pure Au and Hg cluster properties. *Physical Chemistry Chemical Physics*. 13 - 46, pp. 20863 - 20870. 2011.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.573
Position of publication: 5
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
No. of journals in the cat.: 33
Citations: 18
- 22** MB Torres; EM Fernandez; LC Balbas. Study of the Structural and Electronic Properties of [Ti@Si-16](n), [Sc@Si16K](n), and [V@Si16F](n) (n ≤ 9) Aggregates from First Principles. *Journal of Physical Chemistry C*. 115 - 2, pp. 335 - 350. 2011.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 4.805
Position of publication: 26
Source of citations: WOS
Format: Journal
Category: Science Edition - CHEMISTRY, PHYSICAL
Journal in the top 25%: Yes
No. of journals in the cat.: 26
Citations: 14
- 23** MB Torres; EM Fernandez; LC Balbas. Theoretical Study of the Structural and Electronic Properties of Aggregates, Wires, and Bulk Phases Formed from M@Si-16 Superatoms (M = Sc-, Ti, V+). *International Journal of Quantum Chemistry*. 111 - 2, pp. 444 - 462. 2011.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.357
Position of publication: 22
Source of citations: WOS
Format: Journal
Category: MATHEMATICS, INTERDISCIPLINARY APPLICATIONS
Journal in the top 25%: No
No. of journals in the cat.: 95
Citations: 10



- 24** EM Fernandez; E Chacon; P Tarazona. Thickness and fluctuations of free and adsorbed liquid films. *Physical Review B*. 84 - 20, pp. 205435. 2011.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.691
Position of publication: 13
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, CONDENSED MATTER
Journal in the top 25%: Yes
No. of journals in the cat.: 69
Citations: 7
- 25** GL Lurrabaquiu; MB Torres; EM Fernandez; LC Balbas. Trends in the formation of aggregates and crystals from M@Si-16 clusters: a study from first principle calculations. *Journal of Mathematical Chemistry*. 48 - 1, pp. 109 - 117. 2010.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.259
Position of publication: 70
Source of citations: WOS
Format: Journal
Category: CHEMISTRY, MULTIDISCIPLINARY
Journal in the top 25%: No
No. of journals in the cat.: 147
Citations: 1
- 26** E Chacon; EM Fernandez; D Duque; R Delgado-Buscalioni; P Tarazona. Comparative study of the surface layer density of liquid surfaces. *Physical Review B*. 80 - 19, pp. 195403. 2009.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 3.475
Position of publication: 12
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, CONDENSED MATTER
Journal in the top 25%: Yes
No. of journals in the cat.: 12
Citations: 25
- 27** JI Martinez; EM Fernandez. Optical absorption spectra of Ag-11 isomers. *European Physical Journal D*. 52 - 1-3, pp. 199 - 202. 2009.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.420
Position of publication: 20
Source of citations: WOS
Format: Journal
Category: PHYSICS, ATOMIC, MOLECULAR & CHEMICA
Journal in the top 25%: No
No. of journals in the cat.: 33
Citations: 6
- 28** EM Fernandez; MB Torres; LC Balbas. Theoretical study of the coadsorption of CO and O-2 on doped cationic gold clusters MAun+ (M = Ti, Fe, Au; n=1, 6, 7). *European Physical Journal D*. 52 - 1-3, pp. 135 - 138. 2009.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.420
Position of publication: 20
Source of citations: WOS
Format: Journal
Category: PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: No
No. of journals in the cat.: 33
Citations: 9



- 29** MB Torres; EM Fernandez; LC Balbas. Theoretical study of oxygen adsorption on pure Au-n+1(+) and doped MAun+ cationic gold clusters for M = Ti, Fe and n=3-7. JOURNAL OF PHYSICAL CHEMISTRY A. 112 - 29, pp. 6678 - 6689. 2008.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 2.871
Position of publication: 7
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: Yes
No. of journals in the cat.: 7
Citations: 41
- 30** EM Fernandez; RI Eglitis; G Borstel; LC Balbas. Ab initio calculations of H₂O and O-2 adsorption on Al₂O₃ substrates. COMPUTATIONAL MATERIALS SCIENCE. 39 - 3, pp. 587 - 592. 2007.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.135
Position of publication: 80
Source of citations: WOS
Format: Journal
Category: Science Edition - MATERIALS SCIENCE, MULTIDISCIPLINARY
Journal in the top 25%: No
No. of journals in the cat.: 80
Citations: 39
- 31** EM Fernandez; LC Balbas. Theoretical study of CO adsorption on Au/alumina substrates. PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE. 203 - 6, pp. 1277 - 1283. 2006.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.211
Position of publication: 70
Source of citations: WOS
Format: Journal
Category: MATERIALS SCIENCE, MULTIDISCIPLINARY
Journal in the top 25%: No
No. of journals in the cat.: 70
Citations: 5
- 32** EM Fernandez; R Eglitis; G Borstel; LC Balbas. Adsorption and dissociation of water on relaxed alumina clusters: a first principles study. PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS. 242 - 4, pp. 807 - 809. 2005.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 0.836
Position of publication: 36
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, CONDENSED MATTER
Journal in the top 25%: No
No. of journals in the cat.: 36
Citations: 11
- 33** MB Torres; EM Fernandez; LC Balbas. Density functional study of the stability and magnetic behaviour of Au_nTM⁺ clusters (TM = An, Sc, Ti, V, Cr, Mn, Fe; 1 ≤ n ≤ 9). PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS. 242 - 4, pp. 819 - 821. 2005.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 0.836
Position of publication: 36
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, CONDENSED MATTER
Journal in the top 25%: No
No. of journals in the cat.: 36
Citations: 3



- 34** EM Fernandez; K Michaelian; LC Balbas; LA Perez; IL Garzon. Structural properties of bimetallic clusters from density functional calculations. INTERNATIONAL JOURNAL OF MODERN PHYSICS B. 19 - 15-17, pp. 2339 - 2344. 2005.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 0.381
Position of publication: 51
Source of citations: WOS
Format: Journal
Category: Science Edition - PHYSICS, CONDENSED MATTER
Journal in the top 25%: No
No. of journals in the cat.: 51
Citations: 26
- 35** EM Fernandez; JM Soler; IL Garzon; LC Balbas. Trends in the structure and bonding of neutral and charged noble metal clusters. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 101 - 6, pp. 740 - 745. 2005.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.192
Position of publication: 27
Source of citations: WOS
Format: Journal
Category: Science Edition - MATHEMATICS, INTERDISCIPLINARY APPLICATIONS
Journal in the top 25%: No
No. of journals in the cat.: 27
Citations: 24
- 36** EM Fernandez; MB Torres; LC Balbas. Trends in the bonding of the first-row transition metal compounds: V(001) surface, TM-oxide and nitride molecules, and AunTi ($2 \leq n \leq 7$) clusters. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY. 99 - 1, pp. 39 - 46. 2004.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.392
Position of publication: 17
Source of citations: WOS
Format: Journal
Category: Science Edition - MATHEMATICS, INTERDISCIPLINARY APPLICATIONS
Journal in the top 25%: No
No. of journals in the cat.: 17
Citations: 17
- 37** EM Fernandez; G Borstel; JM Soler; LC Balbas. Study of $(Al_2O_3)_n(O-x)$ clusters with $n \leq 16$ and $x=0, 1, 2$ from first principles calculations. European Physical Journal D. 24 - 1-3, pp. 245 - 248. 2003.
Type of production: Scientific paper
Impact source: ISI
Impact index in year of publication: 1.612
Position of publication: 14
Source of citations: WOS
Format: Journal
Category: PHYSICS, ATOMIC, MOLECULAR & CHEMICAL
Journal in the top 25%: No
No. of journals in the cat.: 33
Citations: 11
- 38** EM Fernandez; MB Torres; LC Balbas. Density functional studies of noble metal clusters. Adsorption of O-2 and CO on gold and silver clusters. Recent Advances in the Theory of Chemical and Physical Systems. 15, pp. 407 - 432. 2006.
Type of production: Book chapter
Source of citations: WOS
Format: Book
Citations: 6



Works submitted to national or international conferences

- 1** **Title of the work:** Multiple adsorption of molecular oxygen on small Au/Pd cationic clusters at finite temperature. A van der Waals density functional study
Name of the conference: ISSPIC XVIII
Corresponding author: Yes
City of event: Jyvaskyla, Finland
Date of event: 14/08/2016
City organizing entity: Universidad de Jyvaskyla, Finland
E. M. Fernández; L. C. Balbás.
- 2** **Title of the work:** Intrinsic Fluid Interfaces and Non-Locality
Name of the conference: International Conference Statistical Physics
City of event: Rhodes, Greece
Date of event: 07/07/2014
End date: 11/07/2014
Organising entity: Politecnico di Torino
City organizing entity: Italy
E. M. Fernández; E. Chacón; P. Tarazona; A. O. Parry; C. Rascón. "Intrinsic Fluid Interfaces and Non-Locality".
- 3** **Title of the work:** Study of The H₂ Physisorption on (TM@Si₁₆F)₆ Clusters and Wires: Contribution of The Van Der Waals Dispersion Forces
Name of the conference: International Congress on Energy Efficiency and Energy Related Materials
City of event: Antalya, Turkey
Date of event: 2013
End date: 2013
Organising entity: Gebze Institute of Technology
E. M. Fernández; L. C. Balbás.
- 4** **Title of the work:** Theoretical study of Al_{n+1}⁺ clusters and their interaction with Ar
Name of the conference: ISSPIC XVI
Type of participation: 'Participatory - poster
City of event: Leuven, Belgium
Date of event: 2012
E. M. Fernández; L. C. Balbás.
- 5** **Title of the work:** Fluctuaciones de Películas Adsorbidas
Name of the conference: FISES11
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Barcelona, Spain
Date of event: 2011
E. M. Fernández; E. Chacón; P. Tarazona.
- 6** **Title of the work:** H₂ and H₂O adsorption by [TM@Si₁₆F]₆ nanotubes from DFT
Name of the conference: ISMPC11
Type of event: Conference
Type of participation: 'Participatory - poster



Date of event: 2011

City organizing entity: Jyväskylä, Finland

E. M. Fernández; H. Cantera-López; L. C. Balbás; G. Borstel.

7 Title of the work: Thickness and compressibility on free and adsorbed liquid films

Name of the conference: LMC8

Type of participation: 'Participatory - poster

City of event: Viena,

Date of event: 2011

E. M. Fernández; E. Chacón; P. Tarazona.

8 Title of the work: Static polarizability of Ar-AuX complexes (X = F, Hg) and Aun clusters. DFT calculations with a non local correlation van der Waals functional compared to GGA results.

Name of the conference: ISSPIC XV

Type of event: Conference

Type of participation: Participatory - oral communication

City of event: Oaxaca, Mexico

Date of event: 2010

Organising entity: Universidad Nacional Autonoma de Mexico

E. M. Fernández; L. C. Balbás.

9 Title of the work: First principles study of CO adsorption-CO₂ desorption mechanisms on MAu⁻ⁿOm⁺ (M = Ti, Fe; n = 1, 4-7; m = 1-2) clusters.

Name of the conference: ICTAC 13

Type of event: Conference

Type of participation: 'Participatory - poster

Date of event: 2010

City organizing entity: Sendai, Japan

E. M. Fernández; M. B. Torres; L. C. Balbás. 2010.

10 Title of the work: First principles calculation of CO adsorption on MAun⁺-O₂ doped cationic gold-oxygen complexes for m = Ti, Fe (n=3-7).

Name of the conference: XIV EUROPACAT IX.

Type of event: Conference

Type of participation: 'Participatory - poster

Date of event: 2009

City organizing entity: Salamanca, Spain

E. M. Fernández; M. B. Torres; L. C. balbás. 2009.

11 Title of the work: First principles calculation of co adsorption on MAun⁺-O₂ doped cationic gold-oxygen complexes for M =Ti, Fe (n=3-7).

Name of the conference: FPMPMO-2009.

Type of event: Conference

Type of participation: 'Participatory - poster

Date of event: 2009

City organizing entity: Madrid, Spain

E. M. Fernández; M. B. Torres; L. C. Balbás. 2009.

12 Title of the work: Aplicación del ISM al estudio de la transición de mojado

Name of the conference: FISES09

Type of participation: Participatory - oral communication



City of event: Huelva, Spain
Date of event: 2009
E. M. Fernández; E. Chacón; P. Tarazona.

- 13** **Title of the work:** Scaling Relations for Adsorption Energies on Transition Metal Oxide, Sulfide and Nitride surfaces
Name of the conference: 12th International Conference on Theoretical Aspects of Catalysis
Type of participation: 'Participatory - poster
City of event: Varna, Bulgaria
Date of event: 2008
E. M. Fernández, P. G. Moses, A. Toftelund, H. A. Hansen, J. I. Martínez, F. Abild-Pedersen, J. Klei.
- 14** **Title of the work:** Study of the stability of crystals formed by Si₁₆Ti, Si₁₆ScK, and Si₁₆VF super-atom units.
Name of the conference: XIV International Symposium on Small Particles and Inorganic Cluster (ISSPIC)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2008
M. B. Torres; E. M. Fernández; L. C. Balbás.
- 15** **Title of the work:** Theoretical study of oxygen adsorption on pure Auⁿ⁺¹⁺ and doped MAuⁿ⁺ cationic gold cluster for M = Ti, Fe (n =3-7). Is it viable the co-adsorption of CO and O₂ on MAu₇⁺?
Name of the conference: XIV International Symposium on Small Particles and Inorganic Cluster (ISSPIC)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2008
M. B. Torres, E. M. Fernández y L. C. Balbás.
- 16** **Title of the work:** Trends in the formation of aggregates of silicon doped super-molecular units
Name of the conference: XIV International Symposium on Small Particles and Inorganic Cluster (ISSPIC)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2008
M. B. Torres; G. López; E. M. Fernández; L. C. Balbás.
- 17** **Title of the work:** Density Functional Calculations of Ammonia Synthesis on gamma-Mo₂N
Name of the conference: Europacat VIII
Type of participation: 'Participatory - poster
City of event: Turku, Finland
Date of event: 2007
E. M. Fernández; T. Bligaard; J. K. Nørskov.
- 18** **Title of the work:** Electrocatalysis at the sub-nanometer scale: Structure and function of supported Mo₃S₄+4 cluster
Name of the conference: NanoDay
Type of participation: 'Participatory - poster
City of event: Lingby, Denmark
Date of event: 2006
T. F. Jaramillo, S. Saadi, E. M. Fernández, J. Zhang, B. L. Ooi, J. Bonde, J. Ulstrup, J. K. Nørskov.



- 19** **Title of the work:** Density functional Studies of noble metal clusters. Adsorption of O₂ and CO on gold and silver clusters
Name of the conference: Symposium on Size Selected clusters (S3C)
Type of event: Conference
Type of participation: 'Participatory - poster
City of event: Brand,
Date of event: 2005
E. M. Fernández; M. B. Torres; L. C. Balbás.
- 20** **Title of the work:** First principles study of the size dependent selective behaviour of O₂ adsorption on free silver and gold clusters
Name of the conference: 7th Iberian Joint Meeting on Atomic and Molecular Physics
Type of participation: 'Participatory - poster
City of event: Lisboa, Portugal
Date of event: 2005
M. B. Torres; E. M. Fernández; L. C. Balbás.
- 21** **Title of the work:** O₂ adsorption on cationic gold clusters pure and doped with a 3d transition metal
Name of the conference: XXX Reunión bienal de la Real Sociedad Española de Física
Type of participation: Participatory - oral communication
Date of event: 2005
M. B. Torres; E. M. Fernández; L. C. Balbás.
- 22** **Title of the work:** Theoretical study of O₂ and CO adsorption on gold clusters in gas phase and supported on alumina nano-particles and surfaces
Name of the conference: X-th Symposium on Surface Physics (SSP10)
Type of participation: Participatory - oral communication
City of event: Praga, Czech Republic
Date of event: 2005
E. M. Fernández; L. C. Balbás.
- 23** **Title of the work:** Theoretical study of O₂ and CO adsorption on gold clusters in gas phase and supported on alumina nano-particles and surfaces
Name of the conference: XXX Reunión bienal de la Real Sociedad Española de Física
Type of participation: Participatory - oral communication
City of event: Orense, Spain
Date of event: 2005
E. M. Fernández; L. C. Balbás.
- 24** **Title of the work:** Theoretical study of O₂ and CO adsorption on gold clusters in gas phase and supported on alumina nano-particles and surfaces
Name of the conference: Theoretical Biophysics Symposium (TEOBIO05)
Type of participation: 'Participatory - poster
City of event: Orebrö, Sweden
Date of event: 2005
E. M. Fernández; L. C. Balbás.
- 25** **Title of the work:** Theoretical study of O₂ and CO adsorption on gold clusters in gas phase and supported on alumina nano-particles and surfaces
Name of the conference: Trends in Nanotechnology (TNT-2005)
Type of participation: 'Participatory - poster



City of event: Oviedo, Spain
Date of event: 2005
E. M. Fernández; L. C. Balbás.

- 26** **Title of the work:** Adsorption and dissociation of water on nonideal surface of alumina. A first principle study
Name of the conference: IX European conference on organised films (ECOF)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2004
E. M. Fernández; R. Eglitis; G. Borstel; L. C. Balbás.
- 27** **Title of the work:** Adsorption and dissociation of water on relaxed alumina clusters: a first principle study
Name of the conference: Electronic structure principles and applications (ESPA)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2004
E. M. Fernández; R. Eglitis; G. Borstel; L. C. Balbás .
- 28** **Title of the work:** Density functional study if the electronic delocalization and magnetic behaviour in $AunX+$ ($x= Sc, Ti, V, Cr, Mn, Fe; n \leq 9$) clusters.
Name of the conference: IX European conference on organised films (ECOF)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2004
M. B. Torres; E. M. Fernández; L. C. Balbás.
- 29** **Title of the work:** Golden fullerenes? A first principle study of $Au_{18}, Au_{20}, Au_{32}, Au_{50}, Au_{162}$ and Au_{1982} -metal cluster
Name of the conference: Electronic structure principles and applications (ESPA)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2004
E. M. Fernández; J. M. Soler; I. L. Garzón; L. C. Balbás.
- 30** **Title of the work:** Size dependent selective behavior of O_2 on free silver cluster anions. A first principles study
Name of the conference: Electronic structure principles and applications (ESPA)
Type of participation: 'Participatory - poster
City of event: Valladolid, Spain
Date of event: 2004
M. B. Torres; E. M. Fernández; L. C. Balbás.
- 31** **Title of the work:** Structural properties of bimetallic clusters from density functional calculations
Name of the conference: XII International Symposium on Small Particles and Inorganic Cluster (ISSPIC).
City of event: Nanjung, China
Date of event: 2004
E. M. Fernández; J. M. Soler; I. L. Garzón; L. C. Balbás .
- 32** **Title of the work:** Trends in the structure and bonding of neutral and charged noble metal clusters
Name of the conference: Siesta meetig
Type of participation: Participatory - oral communication



City of event: Madrid, Spain

Date of event: 2004

E. M. Fernández; J. M. Soler; I. L. Garzón; L. C. Balbás.

- 33** **Title of the work:** Trends in the structure and bonding of neutral and charged noble metal clusters
Name of the conference: Electronic structure simulations of nanostructures
Type of participation: 'Participatory - poster
City of event: Jyväskylä, Finland
Date of event: 2004
E. M. Fernández; J. M. Soler; I. L. Garzón; L. C. Balbás .
- 34** **Title of the work:** Trends in the structure and bonding of pure and doped noble metal clusters. Application to O₂ and CO adsorption
Name of the conference: Quantum system in chemistry & physics
Type of participation: Participatory - invited/keynote talk
City of event: Les Houches, France
Date of event: 2004
E. M. Fernández; L. C. Balbás.
- 35** **Title of the work:** Tendencias en la estructura atómica y enlace químico de agregados neutros y cargados de metales nobles
Name of the conference: Segunda reunión mexicana de físico-química teórica
Type of participation: Participatory - oral communication
City of event: Guanajuato, Mexico
Date of event: 2003
E. M. Fernández; I. L. Garzón; L. C. Balbás.
- 36** **Title of the work:** Tendencias en la estructura atómica y enlace químico de agregados neutros y cargados de metales nobles
Name of the conference: XLVI Congreso nacional de física
Type of participation: 'Participatory - poster
City of event: Mérida, Mexico
Date of event: 2003
E. M. Fernández; I. L. Garzón; L. C. Balbás.
- 37** **Title of the work:** Trends in the bonding of the first-row transition metal compounds: V (001) surface, TM-oxide and nitride molecules and Au_nTi (2 < n < 7) clusters.
Name of the conference: Density functional theory in chemistry and physics (DFT-03)
Type of participation: 'Participatory - poster
City of event: Bruselas,
Date of event: 2003
M. B. Torres; E. M. Fernández; L. C. Balbás.
- 38** **Title of the work:** Trends in the structure and bonding of neutral and charged noble metal clusters
Name of the conference: Second European school on computational chemistry, reaction and molecular dynamics
Type of participation: Participatory - oral communication
City of event: Barcelona, Spain
Date of event: 2003
E. M. Fernández; L. C. Balbás.



- 39 Title of the work:** Trends in the structure and bonding of neutral and charged noble metal clusters
Name of the conference: Density functional theory in chemistry and physics (DFT-03)
Type of participation: 'Participatory - poster
City of event: Bruselas,
Date of event: 2003
E. M. Fernández; J. M. Soler; I. L. Garzón; L. C. Balbás .
- 40 Title of the work:** Trends in the structure and bonding of neutral and charged noble metal clusters.
Name of the conference: XXIX Reunión bienal de la Real Sociedad Española de Física PUBLICACIÓN: Conference Proceedings: Vol. I, p.226-227 Ed. L. Vázquez, 2002 ISBN=84-655-2771-9
Type of participation: 'Participatory - poster
City of event: Madrid, Spain
Date of event: 2003
E. M. Fernández; J. M. Soler; I. Seijo; I. L. Garzón; L. C. Balbás .
- 41 Title of the work:** First principles calculation of the geometric and electronic structure of $(Al_2O_3)_n(O_x)$ clusters with $n < 15$ and $x=0,1,2$.
Name of the conference: E-MRS spring meeting 2002
Type of participation: 'Participatory - poster
City of event: Strasbourg, France
Date of event: 2002
E. M. Fernández; G. Borstel; J. M. Soler; L. C. Balbás.
- 42 Title of the work:** Study of $(Al_2O_3)_n(O_x)$ clusters with $n < 16$ and $x = 0,1,2$ from first principles calculation.
Name of the conference: XI International Symposium on Small Particles and Inorganic Cluster (ISSPIC) PUBLICACIÓN: Coference Proceedings: J-9
Type of participation: 'Participatory - poster
City of event: Strasbourg, France
Date of event: 2002
E. M. Fernández; G. Borstel; J. M. Soler; L. C. Balbás.

Other dissemination activities

- 1 Title of the work:** Nanoagregados: ¿Solución al almacenamiento de Hidrógeno?
Name of the event: Proyecto STEM Talent Girl Valladolid
Type of event: Conferences given
City of event: Valladolid, 02/02/2019, Spain
Date of event: 02/02/2019
Organising entity: Proyecto STEM Talent Girl
Eva M. Fernández.
- 2 Title of the work:** Nanoagregados: ¿Solución al almacenamiento de Hidrógeno?
Name of the event: Celebración día San Alberto Facultad de Ciencias
Type of event: Conferences given
City of event: Madrid, 15/11/2018, Spain
Date of event: 15/11/2018
Organising entity: Facultad de Ciencias, UNED
Eva M. Fernández.



- 3 Title of the work:** Organización de la Semana de la Ciencia (Universidad de Valladolid).
Name of the event: Semana de la Ciencia
Type of event: Fairs and exhibitions
City of event: Valladolid, Spain
Date of event: 2011
Organising entity: Universidad de Valladolid **Type of entity:** University

R&D management and participation in scientific committees

Scientific, technical and/or assessment committees

Committee title: Consejo editorial de la Real Sociedad Española de Física
Start date: 01/09/2018

Evaluation and revision of R&D projects and articles

- 1 Performed tasks:** Evaluadora de proyectos para la Universidad de Leuven (Bélgica)
Entity where activity was carried out: Universidad de Leuven **Type of entity:** University
City of entity: Belgium
Start-End date: 2013 - 2013
- 2 Performed tasks:** Referee of The European Physical Journal D
Entity where activity was carried out: Springer
Start date: 2006
- 3 Performed tasks:** Referee of the Journal of Physical Chemistry
Entity where activity was carried out: ACS
Start date: 2006

Other achievements

Stays in public or private R&D centres

- 1 Entity:** Instituto de Ciencia de los Materiales de Madrid
City of entity: Madrid, Spain
Start-End date: 16/03/2008 - 31/10/2012 **Duration:** 2 years - 7 months - 15 days
Goals of the stay: Post-doctoral
- 2 Entity:** Technical University of Denmark **Type of entity:** University
City of entity: Lyngby, Denmark
Start-End date: 01/03/2006 - 29/02/2008 **Duration:** 2 years
Funding entity: Danish Research Agency, Ministry of Science Technology and Innovation
Goals of the stay: Post-doctoral



- 3** **Entity:** Instituto de Ciencia de los Materiales de Barcelona
City of entity: Barcelona, Spain
Start-End date: 01/06/2004 - 10/08/2004
Goals of the stay: Doctorate
Type of entity: State agency
Duration: 2 months - 15 days
- 4** **Entity:** National Autonomous University of Mexico
Faculty, institute or centre: Institute of Physics
City of entity: Mexico, Mexico
Start-End date: 18/09/2003 - 12/12/2003
Goals of the stay: Doctorate
Type of entity: University
Duration: 2 months - 25 days
- 5** **Entity:** Universidad Autónoma de Madrid
Faculty, institute or centre: Facultad de Ciencias
City of entity: Madrid, Spain
Start-End date: 01/10/2002 - 20/12/2002
Goals of the stay: Doctorate
Type of entity: University
Duration: 2 months - 20 days

Obtained grants and scholarships

- 1** **Name of the grant:** Contrato Ramón y Cajal
Aims: Post-doctoral
Awarding entity: Ministerio Economía y Competitividad
Conferral date: 01/11/2015
End date: 31/10/2020
Type of entity: Ministerio
Duration: 5 years
- 2** **Name of the grant:** Competitive PostDoc contract funded by UNED
Aims: Post-doctoral
Awarding entity: Universidad Nacional de Educación a Distancia
Conferral date: 01/11/2012
End date: 31/10/2016
Type of entity: University
Duration: 4 years
- 3** **Name of the grant:** Comunidad de Madrid contract associated to project
Aims: Post-doctoral
Awarding entity: Comunidad de Madrid
Conferral date: 01/01/2011
End date: 31/10/2012
Type of entity: Public Administration
Duration: 2 years
- 4** **Name of the grant:** PostDoc contract funded by "Junta para la Ampliación de estudios" JaeDoc
Aims: Post-doctoral
Awarding entity: Consejo Superior de Investigaciones Científicas
Conferral date: 15/03/2008
End date: 31/12/2010
Type of entity: State agency
Duration: 3 years
- 5** **Name of the grant:** Danish Research Agency contract associated to project
Aims: Post-doctoral
Awarding entity: Danish Research Agency



Conferral date: 01/03/2006
End date: 29/02/2008

Duration: 2 years

6 Name of the grant: Formación del Personal Universitario (FPU)

Aims: Pre-doctoral

Awarding entity: Dirección Provincial del Ministerio de Educación y Cultura

Type of entity: Publico

Conferral date: 01/01/2002

Duration: 4 years

End date: 31/12/2005

7 Name of the grant: Ayuda a la asistencia a cursos para el desarrollo de la Tesis Doctoral: pago de la inscripción y el transporte

City awarding entity:

Aims: Pre-doctoral

Awarding entity: Universidad de Valladolid

Type of entity: University

Amount of the grant: 574,89 €

Conferral date: 2005

8 Name of the grant: Ayuda a la asistencia a cursos para el desarrollo de la Tesis Doctoral: pago de la inscripción y el transporte

City awarding entity:

Aims: Pre-doctoral

Awarding entity: Universidad de Valladolid

Type of entity: University

Amount of the grant: 725,8 €

Conferral date: 2004

Scientific societies and professional associations

1 Name of the society: Asociación de mujeres investigadoras y tecnólogas

City affiliation entity: Spain

Start date: 01/01/2018

2 Name of the society: Real Sociedad Española de Física

City affiliation entity: Madrid, Spain

Start date: 01/06/2004

Prizes, mentions and distinctions

1 Description: Premios a la Investigación L'oréal-Unesco For Women In Science (Spain)

Awarding entity: L'ORÉAL

Type of entity: Business

Conferral date: 23/11/2017

2 Description: Premio Extraordinario de Doctorado

Awarding entity: Universidad de Valladolid

Type of entity: University

Conferral date: 2007

3 Description: Premio de Real Sociedad Española de Física - Fundación BBVA para Investigadores Noveles en Física Teórica

Awarding entity: Real Sociedad Española de Física - Fundación BBVA



Conferral date: 2007

Obtained accreditations/recognitions

- 1** **Description:** Acreditación como Profesor Titular de Universidad
Accrediting entity: Agencia Nacional de Evaluación de la Calidad y Acreditación **Type of entity:** Public Administration
Date of recognition: 08/03/2018
- 2** **Description:** Acreditación como Profesor Contratado doctor
Accrediting entity: Agencia Nacional de Evaluación de la Calidad y Acreditación **Type of entity:** Public Administration
Date of recognition: 20/10/2011
- 3** **Description:** Acreditación como Profesor de Universidad Privada
Accrediting entity: Agencia Nacional de Evaluación de la Calidad y Acreditación **Type of entity:** Publica
Date of recognition: 20/10/2011
- 4** **Description:** Acreditación como Profesor Ayudante Doctor
Accrediting entity: Agencia de Calidad, Acreditacion y Prospectiva de las Universidades de Madrid **Type of entity:** Publico
City accrediting entity: Madrid, Community of Madrid, Spain
Date of recognition: 07/04/2011
- 5** **Description:** Acreditación como Profesor Contratado doctor
Accrediting entity: Agencia de Calidad, Acreditacion y Prospectiva de las Universidades de Madrid **Type of entity:** Publico
City accrediting entity: Madrid, Community of Madrid, Spain
Date of recognition: 07/04/2011
- 6** **Description:** Acreditación como Profesor de Universidad Privada
Accrediting entity: Agencia de Calidad, Acreditacion y Prospectiva de las Universidades de Madrid **Type of entity:** Publico
City accrediting entity: Madrid, Community of Madrid, Spain
Date of recognition: 07/04/2011
- 7** **Description:** Acreditación como Profesor Ayudante Doctor
Accrediting entity: Agencia Nacional de Evaluación de la Calidad y Acreditación **Type of entity:** Publica
Date of recognition: 25/05/2010



Summary of other achievements

- 1 Description of the achievement:** Estancia Universidad de Osnabrück (Alemania) 10 days in May 2005
City accrediting entity: Osnabrück,
- 2 Description of the achievement:** Estancia Universidad de Osnabrück (Alemania) 10 days in November 2004
City accrediting entity: Osnabrück,
- 3 Description of the achievement:** Estancia Universidad de Osnabrück (Alemania) 10 dyas in November 2005
City accrediting entity: Osnabrück,
- 4 Description of the achievement:** Estancia Universidad de Osnabrück (Alemania) 2 weeks in March 2004
City accrediting entity: Osnabrück,
- 5 Description of the achievement:** International research collaboration with the "Universidad Nacional Autónoma de México (UNAM)" from 2003-2005
- 6 Description of the achievement:** International research collaboration with the Technical University of Denmark (Denmark) from 2008 to 2012
- 7 Description of the achievement:** International research collaboration with the University of Osnabruck (Germany) from 2002
- 8 Description of the achievement:** Referee of The European Physical Journal D