CURRÍCULUM VÍTAE NORMALIZADO

Andrea Droghetti

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GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

FECYT FUNDACIÓN ESPAÑOLA PARA LA CIENCIA Y LA TECNOLOGÍA

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.

Andrea Droghetti graduated with a B.Sc. in Physics in 2004 and a M.Sc. in Theoretical Physics in the spring 2007 from the University of Bologna, Italy .

In the autumn 2007, he joined the Computational Spintronics Group in Trinity College Dublin (Ireland), where he finally completed the Ph.D in Physics in 2012 under the supervision of Prof. S. Sanvito. Dr. Droghetti's research focused on electronic structure theory applied to spintronics. He provided for the first time an accurate ab-initio description of small polarons in semiconductors (Phys. Rev. B 78, 140404) and, moreover, he proposed the concept of electrical control over the magnetic state of molecules (Phys. Rev. Lett. 107, 047201).

From 2012 until 2014, Dr. Droghetti worked as a postdoctoral researcher for the EU-project “Next Generation Hybrid Interfaces for Spintronic applications” HINTS. This project aimed at understanding the spin-transport properties of hybrid interfaces between molecules and metals. By collaborating with the experimentalists, Dr. Droghetti proposed a new spin-relaxation mechanism (Nat. Commun. 7, 12668) and he showed that the spin-texture of topological insulators could be modified via molecular adsorption (Nano letters 15, 6022). These results contributed to establish the research direction now called “spinterface” science.

After HINTS and just two years after the Ph.D., Dr. Droghetti became principal investigator (PI) in the collaborative project “Electrical spin manipulation in electroactive molecules” ACMOL (http://acmolproject.eu). ACMOL was funded by the EU through the call for the Young Explores' FET OPEN projects. It started in January 2014 and was completed in December 2016. ACMOL proposed new routes to integrate electroactive molecules and graphene so to overcome the limitations of molecular devices in terms of mechanical and thermal stability, while attaining electrical control over the molecular spin and charge states (Science Advances 3, e1602297). The results represent a step forward in advancing molecular electronics from fundamental science toward technological applications.

In the winter of 2015, Dr. Droghetti moved from Trinity College Dublin to the University of the Basque Country, where he joined the Nano-Bio Spectroscopy Group led by Prof. A. Rubio in San Sebastian. The move was in part supported by the “ayudas para la formación postdoctoral” of the “Ministerio de Economía y Competitividad”. At the University of the Basque Country, Dr. Droghetti kept working as PI in ACMOL, but he also started collaborating with other groups in the San Sebastian research campus on a number problems related to spin-transport in low dimensional systems. After ACMOL, Dr. Droghetti was awarded of the Marie Sklodowska-Curie individual fellowship. The project, SpinMan, which ran from 2016 to 2018 investigated current-induced magnetic excitations in molecules and atoms finally proposing new means for spin-manipulations and quantum operations (Science Advances 3, e1603137).

For the last five years, Dr. Droghetti has relied only upon the funding provided by ACMOL and by individual fellowships in order to carry out independent research. He has supervised a master student, a one-year visiting student and co-supervised a Ph.D. student. He has now become a group leader within the Nano-Bio Spectrocopy Group.

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 number of publications: 25 articles in peered-reviewed journals and 2 book chapters
Total number of citations: 472 (Web of Science), 592 (Google Scholar)
H index: 12 (Web of Science), 13(Google Scholar)

Andrea Droghetti

Surname(s): **Droghetti**
Name: **Andrea**
ORCID: **0000-0003-4106-7327**
ResearcherID: **F-8058-2016**
Personal web page: **http://nano-bio.ehu.es/users/droghetti**

Current professional situation

Employing entity: Universidad del País Vasco **Type of entity:** University
Department: Departamento de Física de Materiales, Unidad de Física de Materiales
Professional category: Postdoc
Start date: 01/03/2015
Type of contract: Temporary **Dedication regime:** Full time
Primary (UNESCO code): 220208 - Magnetism; 220306 - Electron transport; 220607 - Molecular spectroscopy; 220609 - Organic molecules; 221007 - Electronic spectroscopy; 221020 - Molecular spectroscopy; 221023 - Quantum theory; 221028 - Solid state chemistry; 221029 - Solid state physics; 221033 - Transport phenomena; 221110 - Electron states; 221111 - Electron transport properties; 221114 - Interfaces; 221117 - Magnetic properties; 221125 - Semiconductors; 221128 - Surfaces; 221200 - Theoretical physics
Secondary (UNESCO code): 230700 - Physical chemistry
Performed tasks: Andrea Droghetti's research activity has been dedicated to electronic structure theory for materials with relevant applications in electronics and spintronics. He has a consolidated expertise in many theoretical methods, namely Density Functional Theory, Quantum Monte Carlo and Dynamical Mean-Field Theory. In addition, he has been contributing to the development of the electronic transport software Smeagol, which allows to perform ab-initio simulations of nano-devices. In Smeagol, he has implemented novel features to study materials with large spin-orbit coupling and to address quantum many-body effects (e.g. Kondo effect). Among the materials that Andrea Droghetti has investigated so far, there are: organic and inorganic semiconductors, topological insulators, ferromagnetic metals, graphene and other 2-dimensional compounds, magnetic molecules.
Identify key words: Density functional theory; Excited states; Electronic correlation; Electronic; Materials; Defects; Spectroscopy; Interfaces; Quantum hall effect; Excitations; Electronic structure; Fenomenos de no equilibrio [eng]; Transport phenomenon; Phase transition; Kondo models; Magnetism; Transiciones metal-aislante y densidad de carga [eng]; Physics - Quantum physics; Superconductors

Previous positions and activities

	Employing entity	Professional category	Start date
	Trinity College Dublin	Postdoc	01/02/2012

Employing entity: Trinity College Dublin **Type of entity:** University
Professional category: Postdoc
Start-End date: 01/02/2012 - 31/01/2015

Education

University education

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

1 **University degree:** Higher degree
Name of qualification: M.Sc. in Theoretical Physics
Degree awarding entity: University Of Bologna (Italy) **Type of entity:** University
Date of qualification: 23/03/2007

2 **University degree:** Middle degree
Name of qualification: B.Sc. in Physics
Degree awarding entity: University Of Bologna (Italy) **Type of entity:** University
Date of qualification: 10/12/2004

Doctorates

Doctorate programme: Physics
Degree awarding entity: Trnity College Dublin (Ireland)
Date of degree: 29/06/2012

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
German	A1	A1	A1	A1	A1
Spanish	C2	C2	C1	C1	C1
English	C2	C2	C2	C2	C2
Italian	C2	C2	C2	C2	C2

Teaching experience

General teaching experience

1 **Name of the course:** Laboratory of Computational Physics
University degree: Physics
End date: 2011
Entity: Trinity College Dublin (Ireland)

2 **Name of the course:** Laboratory of Physics
University degree: Physics
End date: 2010
Entity: Trinity College Dublin (Ireland)

Experience supervising doctoral thesis and/or final year projects

1 **Project title:** Master equation approach for electronic transport in nanostructures
Entity: Trinity College Dublin (Ireland) **Type of entity:** University
Student: Aurélien Bailly Reyre
Date of reading: 09/2013

2 **Project title:** Magnetic and spin-transport properties of hybrid organic-inorganic interfaces
Entity: Universidad del País Vasco **Type of entity:** University
Student: Jean Pierre Inchaustegui Rovoredo

Student tutorials

1 **Name of the programme:** Mobility programme
Entity: Trinity College Dublin (Ireland)

2 **Name of the programme:** Mobility programme
Entity: Universidad del País Vasco **Type of entity:** University

Other activities/achievements not included above

1 **Description of the activity:** Invited lecture "Overview about Molecular Spintronics" at the Spin+X: Summer School on Molecular Spintronics
Organising entity: University of Mainz (Germany)
End date: 10/2018

2 **Description of the activity:** Invited lecture "First-principles simulations of charge and spin transport in nano-structures"
Organising entity: University of Leeds (UK) **Type of entity:** University
End date: 02/11/2017

Scientific and technological experience

Research and development groups/teams

Name of the group: Cost Action on Molecular Spintronics (MolSpin)
Start date: 2016

Scientific or technological activities

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

1 **Name of the project:** Electrical Spin Manipulation in Atoms and Molecules (Marie Curie Individual Fellowship)
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Andrea Droghetti
Nº of researchers: 1
Funding entity or bodies:
European Commission

Start-End date: 01/09/2016 - 31/08/2018

2 **Name of the project:** The Novel Materials Discovery (NOMAD) Laboratory
Entity where project took place: University of the Basque Country / Max Planck Institute
City of entity: San Sebastian / Hamburg,
Nº of researchers: 100
Funding entity or bodies:
European Commission

Start-End date: 2016 - 2018

3 **Name of the project:** Electrical Spin Manipulation in Electro-Active Molecules (Young Explorers' FET OPEN)
Entity where project took place: Trinity College Dublin / Universidad del Pais Vasco
Name principal investigator (PI, Co-PI....): Andrea Droghetti
Nº of researchers: 8
Funding entity or bodies:
European Commission

Start-End date: 01/01/2014 - 31/12/2016

4 **Name of the project:** Next Generation Hybrid Interfaces for Spintronic Applications
Entity where project took place: Trinity College Dublin **Type of entity:** University
City of entity: Dublin, Ireland
Name principal investigator (PI, Co-PI....): Stefano Sanvito
Nº of researchers: 50

Funding entity or bodies:
European Commission

Start-End date: 01/06/2011 - 31/05/2014

5 **Name of the project:** Magnetic and spin-transport properties of hybrid organic-inorganic interfaces (project for Ph.D. student)
Entity where project took place: Universidad del País Vasco **Type of entity:** University
Name principal investigator (PI, Co-PI....): Andrea Droghetti; Angel Rubio
Nº of researchers: 3
Funding entity or bodies:
Materials Physics Center **Type of entity:** R&D Centre
City funding entity: San Sebastian, Spain

Start date: 2017

6 **Name of the project:** Class A (High-Impact) computational project at the Irish Centre for High End Computing
Name principal investigator (PI, Co-PI....): Andrea Droghetti; Ivan Rungger
Nº of researchers: 2
Start date: 2016

7 **Name of the project:** Class B (Regular) computational project at the Irish Centre for High End Computing
Name principal investigator (PI, Co-PI....): Andrea Droghetti
Nº of researchers: 1
Start date: 2015

Scientific and technological activities

Scientific production

Publications, scientific and technical documents

1 Andrea Droghetti; Wilhelm Appelt; Liviu Chioncel; Milos Radonjic; Enrique Munoz; Stefan Kirchner; Dieter Vollhardt; Ivan Rungger. Predicting the conductance of strongly correlated molecules: the Kondo effect in perchlorotriphenylmethyl/Au junctions. Nanoscale. 10, pp. 17738. 13/09/2018.
Type of production: Scientific paper

2 Francesc Bejarano; Ignacio -Jose Olavarria Contreras; Andrea Droghetti; Ivan Rungger; Alexander Rudnev; Diego Gutiérrez; Marta Mas Torrent; Jaume Veciana; Herre van der Zant; Concepció Rovira; Enrique Burzurí; Núria Crivillers. Robust organic radical molecular junctions using acetylene terminated groups for C-Au bond formation. Journal of the American Chemical Society. 140, pp. 1691. American Chemical Society, 07/01/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes

3 Alexander Rudnev; Veerabhadrarao Kaliginedi; Andrea Droghetti; Hiroaki Ozawa; Akiyoshi Kuzume; Masa-aki Haga; Peter Broekmann; Ivan Rungger. Stable anchoring chemistry for room temperature charge transport through graphite-molecule contacts. Science Advances. 3, pp. e1602297. American Association for the Advancement of Science, 01/06/2017.

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

4 Shichao Yan; Luigi Malavolti; Jacob Burgess; Andrea Droghetti; Angel Rubio; Sebastian Loth. Nonlocally sensing the magnetic states of nanoscale antiferromagnets with an atomic spin sensor. Science Advances. 3, pp. e1603137. American Association for the Advancement of Science, 01/05/2017.
Type of production: Scientific paper **Format:** Journal

5 Andrea Droghetti; Ivan Rungger. Quantum transport simulation scheme including strong correlations and its application to organic radicals adsorbed on gold. Physical Review B. 95, pp. 085131. American Physical Society, 22/02/2017.
Type of production: Scientific paper **Format:** Journal

6 Gonca Seber; Alexander Rudnev; Andrea Droghetti; Ivan Rungger; Jaume Veciana; Marta Mas-Torrent; Concepció Rovira; Núria Crivillers. Covalent modification of highly ordered pyrolytic graphite with a stable organic free radical using diazonium chemistry. Chemistry-A European Journal. 23, pp. 1415. 27/12/2016.
Type of production: Scientific paper **Format:** Journal

7 Alexander V. Rudnev; Carlos Franco; Núria Crivillers; Gonca Seber; Andrea Droghetti; Ivan Rungger; Ilya V. Pobelov; Jaume Veciana; Marta Mas-Torrent; Concepció Rovira. A redox-active radical as an effective nanoelectronic component: stability and electrochemical tunnelling spectroscopy in ionic liquids. Physical Chemistry Chemical Physics. 18, pp. 27733. Royal Society of Chemistry, 26/09/2016.
Type of production: Scientific paper **Format:** Journal

8 Andrea Droghetti; Philip Thielen; Ivan Rungger; Norman Haag; Nicolas Großmann; Johannes Stöckl; Benjamin Stadtmüller; Martin Aeschlimann; Stefano Sanvito; Mirko Cinchetti. Dynamic spin filtering at the Co/Alq3 interface mediated by weakly coupled second layer molecules. Nature Communications. 7, pp. 12668. Nature Research, 31/08/2016.
Type of production: Scientific paper **Format:** Journal

9 Maria Fumanal; Lucas K. Wagner; Stefano Sanvito; Andrea Droghetti. Diffusion Monte Carlo Perspective on the Spin-State Energetics of [Fe (NCH) 6] 2+. Journal of Chemical Theory and Computation. 12, pp. 4233. American Chemical Society, 23/08/2016.
Type of production: Scientific paper **Format:** Journal

10 Andrea Droghetti; Ivan Rungger; Chaitanya Das Pemmaraju; Stefano Sanvito. Fundamental gap of molecular crystals via constrained density functional theory. Physical Review B. 93, pp. 195208. American Physical Society, 16/05/2016.
Type of production: Scientific paper **Format:** Journal

11 Liviu Chioncel; Cristian Morari; Andreas Ostlin; Wilhelm Hans Appelt; Andrea Droghetti; Milos M. Radonjic; Ivan Rungger; Levente Vitos; Ulrich Eckern; Andrei V. Postnikov. Transmission through correlated Cu_n Co Cu_n heterostructures. Physical Review B. 92, pp. 054431. American Physical Society, 24/08/2015.
Type of production: Scientific paper **Format:** Journal

12 Sebastian Jakobs; Awadhesh Narayan; Benjamin Stadtmüller; Andrea Droghetti; Ivan Rungger; Yew S Hor; Svetlana Klyatskaya; Dominik Jungkenn; Johannes Stöckl; Martin Laux; others. Controlling the Spin Texture of Topological Insulators by Rational Design of Organic Molecules. Nano letters. 15, pp. 6022. American Chemical Society, 11/08/2015.
Type of production: Scientific paper **Format:** Journal

13 Andrea Droghetti; Ivan Rungger; Mirko Cinchetti; Stefano Sanvito. Vibron-assisted spin relaxation at a metal/organic interface. Physical Review B. 91, pp. 224427 - 224427. American Physical Society, 24/06/2015.
Type of production: Scientific paper **Format:** Journal

14 Awadhesh Narayan; Ivan Rungger; Droghetti Andrea; Stefano Sanvito. Ab initio transport across bismuth selenide surface barriers. Physical Review B. 90, pp. 205431. American Physical Society, 24/11/2014.
Type of production: Scientific paper **Format:** Journal

15 Andrea Droghetti; Mirko Cinchetti; Stefano Sanvito. Electronic structure of metal quinoline molecules from G 0 W 0 calculations. Physical Review B. 89, pp. 245137. APS, 30/06/2014.
Type of production: Scientific paper **Format:** Journal

16 Andrea Droghetti; Sabine Steil; Nicolas Großmann; Norman Haag; Hongtao Zhang; Maureen Willis; William P. Gillin; Alan J. Drew; Martin Aeschlimann; Stefano Sanvito; Mirko Cinchetti. Electronic and magnetic properties of the interface between metal-quinoline molecules and cobalt. Physical Review B. 89, pp. 094412. American Physical Society, 12/03/2014.
Type of production: Scientific paper **Format:** Journal

17 Sabine Mueller; Sabine Steil; Andrea Droghetti; Nicolas Grossmann; Velimir Meded; Andrea Magri; Bernhard Schaefer; Olaf Fuhr; Stefano Sanvito; Mario Ruben; Mirko Cinchetti; Martin Aeschlimann. Spin-dependent electronic structure of the Co/Al(OP)(3) interface. New Journal of Physics. 15, pp. 113054. 26/11/2013.
Type of production: Scientific paper **Format:** Journal

18 Vasile Chiș; Andrea Droghetti; Radu Isai; Cristian Morari; Ivan Rungger; Stefano Sanvito. DFT structural investigation on Fe (1, 10-phenanthroline) 2 (NCS) 2 spin crossover molecule. AIP Conference Proceedings. 1565, pp. 57. AIP Publishing, 13/11/2013.
Type of production: Scientific paper **Format:** Journal

19 Andrea Droghetti; Dario Alfe; Stefano Sanvito. Ground state of a spin-crossover molecule calculated by diffusion Monte Carlo. Physical Review B. 87, pp. 205114. 13/05/2013.
Type of production: Scientific paper **Format:** Journal

20 Andrea Droghetti; Dario Alfe; Stefano Sanvito. Assessment of density functional theory for iron(II) molecules across the spin-crossover transition. The Journal of Chemical Physics. 137 - 12, pp. 124303. 28/09/2012.
Type of production: Scientific paper **Format:** Journal

21 Andrea Droghetti; Stefano Sanvito. Electric Field Control of Valence Tautomeric Interconversion in Cobalt Dioxolene. Physical Review Letters. 107, pp. 047201. 18/07/2011.
Type of production: Scientific paper **Format:** Journal

22 Andrea Droghetti; Chaitanya Das Pemmaraju; Stefano Sanvito. Polaronic distortion and vacancy-induced magnetism in MgO. Physical Review B. 81, pp. 092403. 01/03/2010.
Type of production: Scientific paper **Format:** Journal

23 Andrea Droghetti; Nadjib Baadji; Stefano Sanvito. MgN: A possible material for spintronic applications. Physical Review B. 80, pp. 235310. 08/12/2009.
Type of production: Scientific paper **Format:** Journal

24 Andrea Droghetti; Stefano Sanvito. Electron doping and magnetic moment formation in N- and C-doped MgO. Applied Physics Letters. 94, pp. 252505. 22/06/2009.
Type of production: Scientific paper **Format:** Journal

25 Andrea Droghetti; Chaitanya Das Pemmaraju; Stefano Sanvito. Predicting d(0) magnetism: Self-interaction correction scheme. Physical Review B. 78, pp. 140404. 17/10/2008.
Type of production: Scientific paper **Format:** Journal

26 Andrea Droghetti; Ivan Rungger. Quantum transport simulations of nano-systems: an introduction to the Green's functions. 21st Century Nanoscience Handbook. Taylor and Francis, 2019.
Type of production: Book chapter **Format:** Book
Corresponding author: Yes

27 Ivan Rungger; Andrea Droghetti; Maria Stamenova. Non-equilibrium Green's functions methods for spin transport and dynamics. Handbook of Materials Modeling. Volume 1 Methods: Theory and Modeling. Springer, 2018.
Type of production: Book chapter **Format:** Book

Works submitted to national or international conferences

1 **Title of the work:** Electron transport including strong correlation effects
Name of the conference: Psi-K workshop "What about U"
City of event: Saragoza, Spain
Date of event: 05/2019
Andrea Droghetti.

2 **Title of the work:** First-principles quantum transport simulations including strong correlation effects
Name of the conference: DPG meeting: Regensburg 2019
City of event: Regensburg, Germany
Date of event: 01/04/2019
Andrea Droghetti.

3 **Title of the work:** Tailoring surface charge and spin transport via molecular and atomic adsorbates (Invited presentation)
Name of the conference: Workshop on "Spins and interfaces"
City of event: Peñíscola, Spain
Date of event: 25/10/2018

4 **Title of the work:** Tailoring charge and spin transport in molecule/layered material interfaces
Name of the conference: International conference on Novel 2D materials explored via scanning probe microscopy & spectroscopy
City of event: Donostia - San Sebastian, Spain
Date of event: 26/06/2018
Andrea Droghetti.

5 **Title of the work:** Charge Transport in Molecular Devices via DFT+DMFT
Name of the conference: APS March Meeting
City of event: Los Angeles, United States of America
Date of event: 05/03/2018
End date: 09/03/2018
Andrea Droghetti; Ivan Rungger; David Jacob; Angel Rubio.

6 **Title of the work:** Tailoring charge and spin transport by hybrid interface design
Name of the conference: European Conference on Molecular Spintronics
City of event: Bologna, Italy
Date of event: 15/11/2016
End date: 18/11/2016
Andrea Droghetti.

7 **Title of the work:** Ballistic spin and charge currents from first-principles simulations
Name of the conference: Interfacial spintronics and spin waves
City of event: San Sebastian, Spain
Date of event: 18/07/2016
End date: 22/07/2016
Andrea Droghetti; Juan Borge; Ilya Tokatly; Angel Rubio.

8 **Title of the work:** Electron transport simulations in the Kondo regime
Name of the conference: Towards reality in modelling of molecular electronics
City of event: San Sebastian, Spain
Date of event: 13/06/2016
End date: 17/06/2016
Andrea Droghetti; Milos Radonjic; Wilhelm Appelt; Liviu Chioncel; Ivan Rungger.

9 **Title of the work:** Electron and spin transport through hybrid organic-inorganic interfaces and in molecular devices: insights from first-principles and model calculations
Name of the conference: ELECSpin 2015 International Workshop on Organic and Graphene Electronics and Spintronics
City of event: Barcelona, Spain
Date of event: 12/03/2015
End date: 13/03/2015
Andrea Droghetti.

10 **Title of the work:** Correlated zero-bias transport in nanostructures
Name of the conference: Strong electron correlation effects in complex d- and f-based magnetic materials for technological applications
City of event: Prague, Czech Republic
Date of event: 01/07/2014
End date: 03/07/2014
Andrea Droghetti.

11 **Title of the work:** Correlated zero-bias transport in graphene and 2D topological insulators nanostructures
Name of the conference: APS March Meeting
City of event: Denver, United States of America
Date of event: 03/03/2014
End date: 07/03/2014
Andrea Droghetti; Awadhesh Narayan; Ivan Rungger; Stefano Sanvito.

12 **Title of the work:** Modelling organic-ferromagnetic interfaces
Name of the conference: European Workshop in Molecular Spintronics
City of event: Puerto Santiago, Tenerife, Canary Islands, Spain
Date of event: 21/11/2013
End date: 24/11/2013
Andrea Droghetti; Ivan Rungger; Mirko Cinchetti; Stefano Sanvito.

13 **Title of the work:** A DFT+model Hamiltonian approach to zero-bias transport in nanostructures: work in progress
Name of the conference: Quantum Monte Carlo in the Apuan Alps VIII
City of event: Vallico di Sotto, Lucca, Italy
Date of event: 27/07/2013

End date: 03/08/2013
Andrea Droghetti; Awadhesh Narayan; Ivan Rungger; Stefano Sanvito.

14 **Title of the work:** Accurate first-principles studies of iron-based molecules
Name of the conference: Joint European Magnetic Symposia
City of event: Parma, Italy
Date of event: 09/09/2012
End date: 14/09/2012
Andrea Droghetti; Dario Alfe; Stefano Sanvito.

15 **Title of the work:** First-principles study of spin-crossover molecules (Invited presentation)
Name of the conference: Quantum Monte Carlo in the Apuan Alps VII
City of event: Vallico di Sotto, Lucca, Italy
Date of event: 28/07/2012
End date: 04/08/2012
Andrea Droghetti; Dario Alfe; Stefano Sanvito.

16 **Title of the work:** Molecular spintronics: playing with spin, electric fields and currents (Invited presentation)
Name of the conference: 15th International Workshop on Computational Electronics
City of event: Madison, United States of America
Date of event: 22/05/2012
End date: 25/05/2012
Andrea Droghetti; Aaron Hurley; Nadjib Baadji; Stefano Sanvito.

17 **Title of the work:** Defect-induced magnetism in oxides
Name of the conference: Computer Simulation of Oxides Workshop
City of event: Dublin, Ireland
Date of event: 09/09/2011
End date: 11/09/2011
Andrea Droghetti; Chaitanya Pemmaraju Das; Stefano Sanvito.

18 **Title of the work:** Ab-initio studies of spin crossover and valence tautometic compounds
Name of the conference: Trends in Spintronics and Nanomagnetism
City of event: Lecce, Italy
Date of event: 23/05/2010
End date: 27/05/2010
Andrea Droghetti; Stefano Sanvito.

19 **Title of the work:** New results in d0 magnets
Name of the conference: EU-Mexico workshop on Oxides for Spin Electronics
City of event: Dublin, Ireland
Date of event: 14/12/2009
Andrea Droghetti; Stefano Sanvito.

20 **Title of the work:** Defect-induced magnetism in oxides
Name of the conference: APS March meeting
City of event: Portland, United States of America
Date of event: 15/03/2009
End date: 19/03/2009
Andrea Droghetti; Chaitanya Das Pemmaraju; Stefano Sanvito.

R&D management and participation in scientific committees

Scientific, technical and/or assessment committees

1 **Committee title:** Evaluation of a collaborative project
Affiliation entity: Deutsche Forschungsgemeinschaft (DFG)
City affiliation entity: Germany
End date: 2018

2 **Committee title:** Veni grant within the Innovational Research Incentives Scheme
Affiliation entity: Netherlands Organisation for Scientific Research (NWO)
City affiliation entity: Holland
End date: 2015

Organization of R&D activities

1 **Title of the activity:** Theoretical methods in molecular spintronics
Type of activity: International conference
City convening entity: San Sebastian, Spain
Start-End date: 17/09/2018 - 21/09/2018

2 **Title of the activity:** ACMOL project meeting
Type of activity: Progress meeting for the EU-funded project Electrical Spin Manipulation in Electroactive Molecules
City convening entity: San Sebastian, Spain
Start-End date: 03/04/2016 - 06/04/2016

R&D management

1 **Name of the activity:** Workshop "Theoretical methods in molecular spintronics"
Type of management: Management of organised events
Performed tasks: Organization of the workshop
Start date: 17/09/2018

2 **Name of the activity:** Electrical Spin Manipulation in Atoms and Molecules (Marie Curie Individual Fellowship)
Type of management: Management of R&D&I actions and projects
Performed tasks: Research Fellow
Entity: Universidad del País Vasco
Type of entity: University
Start date: 01/09/2016
Duration: 2 years

3 **Name of the activity:** Class A project (High Impact)
Type of management: Management of R&D&I actions and projects
Performed tasks: Management of high-end computational resources
Entity: Irish Centre for High End Computing
Start date: 2016

4 **Name of the activity:** Class B project (Regular)
Type of management: Management of R&D&I actions and projects
Performed tasks: Management of high-end computational resources
Entity: Irish Centre for High End Computing
Start date: 2015

5 **Name of the activity:** Electrical spin manipulation in electro-active molecules
Type of management: Management of R&D&I actions and projects
Performed tasks: Principal investigator
Entity: Trinity College Dublin / Universidad del Pais Vasco **Type of entity:** University
Start date: 01/01/2014 **Duration:** 3 years

Other achievements

Stays in public or private R&D centres

1 **Entity:** University of Kaiserslautern
End date: 07/2014
Goals of the stay: Guest

2 **Entity:** University College London
City of entity: London,
End date: 12/2010
Goals of the stay: Guest