



Javier Carrasco Rodriguez

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Summary of CV

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

Dr. Javier Carrasco obtained his PhD in 2006 from the Universitat de Barcelona. His Ph.D thesis was devoted to the theoretical description of point defects in metal oxides using ab initio quantum chemistry methods. In 2007 he joined the Theory Department of the Fritz Haber Institute of the Max Planck Society, Berlin, as an Alexander von Humboldt fellow, working in the area of water-metal interfaces using density functional theory. In 2009 he moved to University College London, London, as a Newton International fellow. During this time he focused his research on the molecular-level understanding of ice formation on metal surfaces. Following this, in 2011 he moved to Instituto de Catálisis y Petroleoquímica del Consejo Superior de Investigaciones Científicas, Madrid, as a Ramón y Cajal fellow. Much of his work during this time was centred upon theoretical catalysis for hydrogen production and hydrogenation of hydrocarbons, as well as the application of van de Waals density functionals to molecular adsorption on metal and oxide surfaces. Since September 2013 he leads the Computational Studies group at the CIC Energigune.

His research aims at understanding important phenomena in surface-, materials-, and nano-science in the power storage field. Using concepts from quantum mechanics, solid state physics, and statistical mechanics, he applies and develops methods and computer simulations to study processes of relevance to energy materials - such as the properties of ion insertion and extraction in electrodes and chemical reactions at surfaces. Rechargeable batteries and fuel cells are major focuses of his work.



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: **88**

Total number of Citations: **4866**

(source: **Web of Science**, 07/09/2021)

ORCID: <http://orcid.org/0000-0003-3117-6933>

ResearcherID: <http://www.researcherid.com/rid/I-5488-2015>

Publons: <https://publons.com/a/1310972>



Javier Carrasco Rodriguez

Surname(s): **Carrasco Rodriguez**
Name: **Javier**
ORCID: **0000-0003-3117-6933**

Current professional situation

Employing entity: CIC Energigune
Professional category: Group Leader
Start date: 01/09/2013
Type of contract: Permanent employment contract
Type of entity: R&D Centre
Dedication regime: Full time

Primary (UNESCO code): 230700 - Physical chemistry

Secondary (UNESCO code): 221128 - Surfaces

Tertiary (UNESCO code): 221001 - Catalysis

Performed tasks: Understanding important phenomena in surface- materials- and nano-science in the power storage field. Concepts from quantum mechanics, solid state physics, and statistical mechanics are applied to study processes of relevance to energy materials - such as the properties of ion insertion and extraction in electrodes and chemical reactions at surfaces. Rechargeable batteries and fuel cells are major focuses of the research activity.

Identify key words: Density functional theory

Previous positions and activities

	Employing entity	Professional category	Start date
	Consejo Superior de Investigaciones Científicas	Ramon y Cajal Fellow	03/2011

Employing entity: Consejo Superior de Investigaciones Científicas
Professional category: Ramon y Cajal Fellow
Start-End date: 03/2011 - 08/2013
Type of entity: State agency
Duration: 2 years - 5 months



Education

University education

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

University degree: Higher degree

Name of qualification: Licenciado en Química

Degree awarding entity: Universitat de Barcelona

Type of entity: University

Date of qualification: 19/07/2002

Average mark: Excellent

Doctorates

Doctorate programme: Química teórica computacional

Degree awarding entity: Universitat de Barcelona

Type of entity: University

Date of degree: 15/12/2006

European doctorate: Yes

Date of certificate: 15/12/2006

Thesis director: Francesc Illas Riera

Thesis co-director: Núria López Alonso

Recognition of quality: Yes

Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
German	A1	A2	A1	A1	A1
Italian	A1	B1	A1	A1	A1
Catalan	C2	C2	C2	C2	C2
English	C2	C2	C2	C2	C2
Spanish	C2	C2	C2	C2	C2

Teaching experience

General teaching experience

Type of teaching: Official teaching

Name of the course: Electrochemical Energy Storage

Type of programme: Master's degree

Type of teaching: In person theory

Type of subject: Optional

University degree: Erasmus Mundus Master in Materials for Storage and Conversion

Start date: 09/12/2021

End date: 19/01/2021

Type of hours/ ECTS credits: Hours



Hours/ECTS credits: 9

Entity: Universidad del País Vasco

Type of entity: University

Faculty, institute or centre: Escuela de Ingeniería de Bilbao

Subject language: English

Experience supervising doctoral thesis and/or final year projects

- 1** **Project title:** First principles simulations of sodium-based battery materials
Type of project: Doctoral thesis
Co-director of thesis: Javier Carrasco
Entity: Universidad del País Vasco **Type of entity:** University
Student: Oier Arcelus Elcorobarrtia
Obtained qualification: Cum laude
Date of reading: 12/11/2019
European doctorate: Yes
- 2** **Project title:** Estudio computacional de baterías: Estructura de óxidos laminares P2- y O3-Na_{0.67}FexMn(1-x)O₂ usando DFT
Type of project: End of course project
Entity: Universidad del País Vasco **Type of entity:** University
City of entity: San Sebastian, Basque Country, Spain
Student: Joseba A. Urrestarazu Larrañaga
Obtained qualification: 10
Date of reading: 07/2018
- 3** **Project title:** Análisis computacional para aplicaciones en baterías: Silicio cristalino como ánodo de baterías de iones de sodio
Type of project: End of course project
Entity: Universidad del País Vasco **Type of entity:** University
City of entity: San Sebastian, Basque Country, Spain
Student: Unai Arrieta Begiristain
Obtained qualification: 10
Date of reading: 07/2017
- 4** **Project title:** Density Functional investigation of the structure and stability of sodium superoxide nanoclusters: Relevance for Na-O₂ batteries
Type of project: Minor thesis
Entity: Universidad del País Vasco **Type of entity:** University
City of entity: San Sebastian, Basque Country, Spain
Student: Oier Arcelus Elcorobarrutia
Date of reading: 07/2015



Scientific and technological experience

Scientific or technological activities

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

- 1** **Name of the project:** Solid state sulfide Based LI-Metal batteries for EV applications - SUBLIME
Geographical area: European Union
Degree of contribution: Researcher
Entity where project took place: CIC Energigune, Centro de Investigacion COOP de Energías Alternativas
City of entity: Miñano, Basque Country, Spain
Name principal investigator (PI, Co-PI...): Thorsten Schnorbus
Nº of researchers: 18
Funding entity or bodies:
Horizon 2020

Name of the programme: H2020-LC-BAT-01-2019-2020
Code according to the funding entity: 875028
Start-End date: 01/05/2020 - 30/04/2024 **Duration:** 4 years
Total amount: 7.892.792,5 €
- 2** **Name of the project:** Towards a self-driving discovery platform for electroactive battery materials - ION-SELF
Type of project: Basic research (including archaeological digs, etc) **Geographical area:** National
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: CIC Energigune, Centro de Investigacion COOP de Energías Alternativas **Type of entity:** Foundation
City of entity: Miñano, Basque Country, Spain
Name principal investigator (PI, Co-PI...): Javier Carrasco
Funding entity or bodies:
Ministerio de Economía y Competitividad **Type of entity:** State agency

Type of participation: Principal investigator
Name of the programme: Programa Estatal de Investigación, Desarrollo e Innovación Orientada a los Retos de la Sociedad
Code according to the funding entity: PID2019-106519RB-I00
Start-End date: 06/2020 - 05/2023 **Duration:** 3 years
Total amount: 217.800 €
- 3** **Name of the project:** Simulación de Baterías de Litio-ion - SIBALI
Type of project: Research and development, including transfer **Geographical area:** National
Degree of contribution: Researcher
Entity where project took place: CIC Energigune, Centro de Investigacion COOP de Energías Alternativas **Type of entity:** Foundation

City of entity: Miñano, Basque Country, Spain

Name principal investigator (PI, Co-PI....): Igor Cantero

Nº of researchers: 24

Funding entity or bodies:

Ministerio de Economía y Competitividad

Type of entity: State agency

Type of participation: Team member

Name of the programme: Programa Estatal de I+D+i Orientada a los Retos de la Sociedad (Retos-Colaboración)

Code according to the funding entity: RTC-2017-6538-3

Start-End date: 06/2018 - 06/2021

Duration: 4 years

Participating entity/entities: Arcelormittal Innovación, Investigación e Inversión S.L.; CIC Energigune; Cegasa Portable Energy S.L.U; Mondragon Goi Eskola Politeknikoa S.COOP; Universidad de Oviedo

Total amount: 156.555,35 €

4 Name of the project: High throughput screening to design future materials for batteries

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

Geographical area: National

Degree of contribution: Coordinator of total project, network or consortium

Entity where project took place: CIC Energigune, Centro de Investigacion COOP de Energías Alternativas

Type of entity: Foundation

City of entity: Miñano, Basque Country, Spain

Name principal investigator (PI, Co-PI....): Javier Carrasco

Nº of researchers: 12

Funding entity or bodies:

Ministerio de Economía y Competitividad

Type of entity: State agency

Type of participation: Principal investigator

Name of the programme: Programa Estatal de Investigación, Desarrollo e Innovación Orientada a los Retos de la Sociedad

Code according to the funding entity: ENE2016-81020-R

Start-End date: 01/2017 - 12/2019

Duration: 3 years

Total amount: 145.200 €

5 Name of the project: Stable Interfaces for Rechargeable Batteries

Geographical area: European Union

Degree of contribution: Researcher

Entity where project took place: CIC Energigune, Centro de Investigacion COOP de Energías Alternativas

City of entity: Miñano, Basque Country, Spain

Name principal investigator (PI, Co-PI....): Laurence Hardwick

Funding entity or bodies:

7th Framework Programme for Research

Name of the programme: FP7-ENERGY-2013-1

Start-End date: 09/2013 - 08/2016

Duration: 3 years

Total amount: 3.237.000 €

6 Name of the project: NanoWGS- Water-gas shift reaction on metal-oxide nanocatalysts for hydrogen production

Geographical area: European Union

Degree of contribution: Scientific coordinator

Entity where project took place: CIC Energigune, Centro de Investigacion COOP de Energías Alternativas



City of entity: Miñano, Basque Country, Spain

Name principal investigator (PI, Co-PI....): Javier Carrasco

Nº of researchers: 1

Funding entity or bodies:

7th Framework Programme for Research

Name of the programme: Marie Curie Actions - Career Integration Grants

Start-End date: 03/2012 - 02/2016

Duration: 4 years

Total amount: 100.000 €

7 Name of the project: Catalizadores nanoestructurados basados en metales no nobles para la producción de hidrógeno libre de CO a partir de etanol

Geographical area: National

Degree of contribution: Researcher

Entity where project took place: Consejo Superior de Investigaciones Científicas

Type of entity: State agency

Name principal investigator (PI, Co-PI....): Arturo Martinez Arias

Nº of researchers: 12

Funding entity or bodies:

Ministerio de Economía y Competitividad

Type of entity: State agency

Name of the programme: PROYECTOS DE INVESTIGACIÓN DEL PLAN NACIONAL, SUBPROGRAMA DE PROYECTOS DE INVESTIGACIÓN FUNDAMENTAL NO ORIENTADA

Start-End date: 01/2013 - 01/2016

Duration: 3 years

Total amount: 254.000 €

8 Name of the project: Modelización ab initio a escala molecular, nanoscópica y macroscópica de materiales de interés tecnológico

Geographical area: National

Degree of contribution: Current university student

Entity where project took place: Universitat de Barcelona

Type of entity: University

City of entity: Barcelona, Catalonia, Spain

Name principal investigator (PI, Co-PI....): Francesc Illas

Funding entity or bodies:

Comisión Interministerial de Ciencia y Tecnología

Type of entity: -

City funding entity: Madrid, Community of Madrid, Spain

Start-End date: 2007 - 2009

9 Name of the project: Projectes de recerca per potenciar els grups de recerca

Geographical area: Regional

Degree of contribution: Current university student

Entity where project took place: Universitat de Barcelona

Type of entity: University

City of entity: Barcelona, Catalonia, Spain

Name principal investigator (PI, Co-PI....): Francesc Illas

Funding entity or bodies:

Consejo Interdepartamental de Investigación e Innovación Tecnológica

Type of entity: -

Start-End date: 2006 - 2009



- 10** **Name of the project:** Predicción ab initio de parámetros derivados de la estructura electrónica en química de materiales. Un punto de partida para la simulación no empírica de propiedades macroscópicas
Geographical area: National
Degree of contribution: Current university student
Entity where project took place: Universitat de Barcelona **Type of entity:** University
City of entity: Barcelona, Catalonia, Spain
Name principal investigator (PI, Co-PI....): Francesc Illas
Funding entity or bodies: Comisión Interministerial de Ciencia y Tecnología **Type of entity:** -
City funding entity: Madrid, Community of Madrid, Spain
Start-End date: 2003 - 2005

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

Name of the project: Combined DFT-BVEL investigations for sulfide type solid electrolytes
Type of project: Industrial research **Entity where project took place:** CIC energiGUNE
Degree of contribution: Coordinator of total project, network or consortium
Entity where project took place: CIC energiGUNE
Name principal investigator (PI, Co-PI....): Montse Casas Cabanas; Javier Carrasco Rodriguez
Nº of researchers: 5
Participating entity/entities: UMICORE N.V.
Funding entity or bodies: UMICORE N.V. **Type of entity:** Business
City funding entity: Olen, Belgium
Start date: 25/11/2019 **Duration:** 1 year - 2 months
Total amount: 163.360 €

Scientific and technological activities

Scientific production

- 1** **H index:** 36
Date of application: 07/09/2021
Fuente de Índice H: WOS
- 2** **H index:** 36
Date of application: 07/09/2021
Fuente de Índice H: SCOPUS

Publications, scientific and technical documents

- 1** Andrey Golov; Javier Carrasco. Molecular-Level Insight into the Interfacial Reactivity and Ionic Conductivity of a Li-Argyrodite Li₆PS₅Cl Solid Electrolyte at Bare and Coated Li-Metal Anodes. ACS APPLIED MATERIALS & INTERFACES. in press, AMER CHEMICAL SOC, 01/09/2021.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 2** Jian Xiang Lian; Javier Carrasco. On the formation and diffusion of oxygen vacancies in non-stoichiometric mixed Co₃-xMnxO₄ spinel structures from first-principles calculations. JOURNAL OF PHYSICS: CONDENSED MATTER. 33, pp. 444002. IOP Publishing Ltd, 23/08/2021.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 3** Mauricio Bonilla; Fabián García Daza; Pierre Ranque; Frederic Aguesse; Javier Carrasco; Elena Akhmatkaya. Unveiling Interfacial Li-Ion Dynamics in Li₇La₃Zr₂O₁₂/PEO(LiTFSI) Composite Polymer-Ceramic Solid Electrolytes for All-Solid-State Lithium Batteries. ACS APPLIED MATERIALS & INTERFACES. 13 - 26, pp. 30653 - 30667. AMER CHEMICAL SOC, 23/06/2021.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 4** Suzanne K. Wallace; Anton S. Bochkarev; Ambroise van Rookeghem; Javier Carrasco; Alexander Shapeev; Natalio Mingo. Free energy of (CoMn_{1-x})₃O₄ mixed phases from machine-learning-enhanced ab initio calculations. PHYSICAL REVIEW MATERIALS. 5, pp. 035402-1 - 035402-14. AMER PHYSICAL SOC, 01/03/2021.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 5** Suzanne K. Wallace; Anton S. Bochkarev; Ambroise van Rookeghem; Javier Carrasco; Alexander Shapeev; Natalio Mingo. Modeling the high-temperature phase coexistence region of mixed transition metal oxides from ab initio calculations. PHYSICAL REVIEW RESEARCH. 3, pp. 013139-1 - 013139-12. AMER PHYSICAL SOC, 12/02/2021.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 6** Leire Meabe; Sergio Rodríguez Peña; María Martínez-Ibañez; Yan Zhang; Elias Lobato; Hegoi Manzano; Michel Armand; Javier Carrasco; Heng Zhang. Insight into the Ionic Transport of Solid Polymer Electrolytes in Polyether and Polyester Blends. JOURNAL OF PHYSICAL CHEMISTRY C. 124, pp. 17981 - 17991. AMER CHEMICAL SOC, 07/2020.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 7** Lixin Qiao; Uxue Oteo; Yan Zhang; Sergio Rodríguez Peña; María Martínez-Ibañez; Alexander Santiago; Rosalía Cid; Leire Meabe; Hegoi Manzano; Javier Carrasco; Heng Zhang; Michel Armand. Trifluoromethyl-free anion for highly stable lithium metal polymer batteries. ENERGY STORAGE MATERIALS. 32, pp. 225 - 233. Elsevier, 07/2020.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No

- 8** Maria Martinez-Ibañez; Eduardo Sanchez-Diez; Lixin Qiao; Leire Meabe; Alexander Santiago; Haijin Zhu; Luke A. O'Dell; Javier Carrasco; Maria Forsyth; Michel Armand; Heng Zhang. Weakly Coordinating Fluorine-Free Polysalt for Single Lithium-Ion Conductive Solid Polymer Electrolytes. BATTERIES & SUPERCAPS. 3, pp. 738 - 746. European Chemical Societies Publishing, 05/2020.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 9** Nagore Ortiz Vitoriano; Idoia Ruiz de Larramendi; Robert L. Sacchi; Iñigo Lozano; Craig A. Bridges; Oier Arcelus; Marina Enterría; Javier Carrasco; Teofilo Rojo; Gabriel M. Veith. Goldilocks and the three glymes: How Na⁺ solvation controls Na–O₂ battery cycling. ENERGY STORAGE MATERIALS. 29, pp. 235 - 245. Elsevier, 04/2020.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 10** Maria Martinez-Ibañez; Eduardo Sanchez-Diez; Lixin Qiao; Yan Zhang; Xabier Judez; Alexander Santiago; Itziar Aldalur; Javier Carrasco; Haijin Zhu; Maria Forsyth; Michel Armand; Heng Zhang. Unprecedented Improvement of Single Li-Ion Conductive Solid Polymer Electrolyte Through Salt Additive. ADVANCED FUNCTIONAL MATERIALS. 30 - 16, pp. 2000455. WILEY-VCH VERLAG GMBH, 02/2020.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 11** Abdelali Zaki; Javier Carrasco; Daniel Bielsa; Abdessamad Faik. Tunable redox temperature of Co_{3-x}Mn_xO₄ (0 ≤ x ≤ 3) continuous solid solution for thermochemical energy storage. ACS APPLIED MATERIALS & INTERFACES. 12 - 6, pp. 7010 - 7020. AMER CHEMICAL SOC, 01/2020.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 12** Lixin Dai; Oier Arcelus; Haixiao Wang; Javier Carrasco; Hengbin Zhang; Wei Zhang; Jun Tang. Embedded 3D Li⁺ channels in a water-in-salt electrolyte to develop flexible supercapacitors and lithium-ion batteries. JOURNAL OF MATERIALS CHEMISTRY A. 7 - 43, pp. 24800 - 24806. Royal Society of Chemistry, 11/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 13** Heng Zhang; Uxue Oteo; Haijin Zhu; Xabier Judez; Maria Martinez-Ibañez; Itziar Aldalur; Eduardo Sanchez-Diez; Chunmei Li; Javier Carrasco; Maria Forsyth; Michel Armand. Enhanced Li-ion conductivity of polymer electrolytes with selective introduction of hydrogen in the anion. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION. 58 - 23, pp. 7829 - 7834. WILEY-VCH VERLAG GMBH, 09/2019. ISSN 1932-7447
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 14** Nagore Ortiz-Vitoriano; Nicholas E. Drewett; Elena Gonzalo; Begoña Acebedo; Francisco J. Bonilla; Juan M. López del Amo; Jennifer H. Stansby; Neeraj Sharma; Oier Lakuntza; Javier Carrasco; Teofilo Rojo. High performance P2 sodium layered oxides: an in-depth study into the effect of rationally selected stoichiometry. JOURNAL OF MATERIALS CHEMISTRY A. 7, pp. 21812 - 21826. Royal Society of Chemistry, 09/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 15** Mauricio R. Bonilla; Fabián A. García Daza; Javier Carrasco; Elena Akhmatkaya. Exploring Li-ion conductivity in cubic, tetragonal and mixed-phase Al-substituted Li₇La₃Zr₂O₁₂ using atomistic simulations and effective medium theory. ACTA MATERIALIA. 175, pp. 426 - 435. Elsevier, 08/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No

- 16** Jian Xie; Javier Carrasco; Rongrong Li; Hangjia Shen; Qiong Chen; Minghui Yang. Novel 3D flower-like micro/nano-structure FeS/N-doped-C composites as advanced cathodes with high lithium storage performances. JOURNAL OF POWER SOURCES. 431, pp. 226 - 231. Elsevier, 08/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 17** Heng Zhang; Fangfang Chen; Oier Lakuntza; Uxue Oteo; Lixin Qiao; Maria Martinez-Ibañez; Haijin Zhu; Javier Carrasco; Maria Forsyth; Michel Armand. Suppressed Mobility of Negative Charges in Polymer Electrolytes with an ether-functionalized Anion. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION. 58, pp. 12070 - 12075. WILEY-V C H VERLAG GMBH, 08/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 18** Heng Zhang; Uxue Oteo; Xabier Judez; Gebrekidan Gebresilassie Eshetu; Maria Martinez-Ibañez; Javier Carrasco; Chunmei Li; Michel Armand. Designer Anion Enabling Solid-State Lithium-Sulfur Batteries. JOULE. 3, pp. 1689 - 1702. ELSEVIER, 07/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 19** Heng Zhang; Xabier Judez; Alexander Santiago; Maria Martinez-Ibañez; Miguel Ángel Muñoz; Javier Carrasco; Chunmei Li; Gebrekidan Gebresilassie Eshetu; Michel Armand. Fluorine-Free Nobel Salt Anion for High-Performance All-Solid-State Lithium-Sulfur Batteries. ADVANCED ENERGY MATERIALS. 9, pp. 1900763. WILEY-V C H VERLAG GMBH, 07/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 20** Maider Zarrabeitia; Elena Gonzalo; Marta Pasqualini; Matteo Ciambezi; Oier Lakuntza; Francesco Nobili; Angela Trapananti; Andrea Di Cicco; Giuliana Aquilanti; Nebil A. Katcho; Juan M. López del Amo; Javier Carrasco; Miguel Ángel Muñoz-Márquez; Teofilo Rojo. Unraveling the role of Ti in the stability of positive layered oxide electrodes for rechargeable Na-ion batteries. JOURNAL OF MATERIALS CHEMISTRY A. 7, pp. 14169 - 14179. Royal Society of Chemistry, 05/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 21** Oier Arcelus; Javier Carrasco. Atomistic Insight into Glide-Driven Phase Transformations in Layered Oxides for Sodium-Ion Batteries: A Case Study on Na_xVO₂. ACS APPLIED MATERIALS & INTERFACES. 11, pp. 12562 - 12569. AMER CHEMICAL SOC, 03/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 22** Nebil A. Katcho; Jesus Carrete; Marine Reynaud; Gwenaelle Rousse; Montse Casas-Cabanas; Natalio Mingo; Juan Rodriguez-Carvajal; Javier Carrasco. An investigation of the structural properties of Li and Na fast ion-conductors using highthroughput bond-valence calculations and machine learning. JOURNAL OF APPLIED CRYSTALLOGRAPHY. 52, pp. 148 - 157. IUCr/Wiley, 01/2019.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 23** Uxue Oteo; Maria Martinez-Ibañez; Itziar Aldalur; Eduardo Sanchez-Diez; Javier Carrasco; Michel Armand; Heng Zhang. Improvement of the cationic transport in polymer electrolytes with (difluoromethanesulfonyl) (trifluoromethanesulfonyl)imide salts. CHEMELECTROCHEM. 6, pp. 1019 - 1022. WILEY-V C H VERLAG GMBH, 01/2019. ISSN 1932-7447
Type of production: Scientific paper **Format:** Journal
Corresponding author: No

- 24** Fabián García Daza; Mauricio Bonilla; Llordes Anna; Javier Carrasco; Elena Akhmatkaya. Atomistic Insight into Ion Transport and Conductivity in Ga/Al-doped Li₇La₃Zr₂O₁₂ Solid Electrolytes. ACS APPLIED MATERIALS & INTERFACES. 11, pp. 753 - 765. AMER CHEMICAL SOC, 12/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 25** Melissa L. Liriano; Amanda M. Larson; Chiara Gattinoni; Javier Carrasco; Ashleigh E. Baber; Emily A. Lewis; Colin J. Murphy; Timothy J. Lawton; Matthew D. Marcinkowski; Andrew J. Therrien; Angelos Michaelides; E. Charles H. Sykes. Chirality at two-dimensional surfaces: A perspective from small molecule alcohol assembly on Au(111). JOURNAL OF CHEMICAL PHYSICS. 149, pp. 034703. AMER INST PHYSICS, 07/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 26** Gebrekidan Gebresilassie Eshetu; Xabier Judez; Chunmei Li; Maria Martinez-Ibañez; Ismael Garcia; Oleksandr Bondarchuk; Javier Carrasco; Lide M. Rodriguez-Martinez; Heng Zhang; Michel Armand. Ultrahigh Performance All Solid-State Lithium Sulfur Batteries: Salt Anion's Chemistry-Induced Anomalous Synergistic Effect. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. 140, pp. 9921 - 9933. AMER CHEMICAL SOC, 07/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 27** Oier Arcelus; Sergey Nikolaev; Javier Carrasco; Igor Solovyev. Magnetism of NaFePO₄ and related polyanionic compounds. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 20, pp. 13497 - 13507. Royal Society of Chemistry, 05/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 28** Heng Zhang; Oier Arcelus; Javier Carrasco. Role of asymmetry in the physicochemical and electrochemical behaviors of perfluorinated sulfonimide anions for lithium batteries: A DFT study. ELECTROCHIMICA ACTA. 280, pp. 290 - 299. Elsevier, 05/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 29** Mauricio R. Bonilla; Ariel Lozano; Bruno Escribano; Javier Carrasco; Elena Akhmatkaya. Revealing the Mechanism of Sodium Diffusion in Na_xFePO₄ Using and Improved Force Field. JOURNAL OF PHYSICAL CHEMISTRY C. 122, pp. 8065 - 8075. AMER CHEMICAL SOC, 04/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 30** Ting Deng; Wei Zhang; Oier Arcelus; Dong Wang; Xiaoyuan Shi; Xiaoyu Zhang; Javier Carrasco; Teofilo Rojo; Weitao Zheng. Vertically Co-Oriented Two Dimensional Metal-organic Frameworks for Packaging Enhanced Supercapacitive Performance. COMMUNICATIONS CHEMISTRY. 1, pp. 6. NATURE PUBLISHING GROUP, 03/2018.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 31** Marine Reynaud; Agnieszka Wizner; Nebil A. Katcho; Laura C. Loaiza; Montserrat Galceran; Javier Carrasco; Teofilo Rojo; Michel Armand; Montse Casas-Cabanas. Sodium vanadium nitridophosphate Na₃V(PO₃)₃N as a high-voltage positive electrode material for Na-ion and Li-ion batteries. ELECTROCHEMISTRY COMMUNICATIONS. 84, pp. 14. Elsevier, 09/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No

- 32** Unai Arrieta; Nebil A. Katcho; Oier Arcelus; Javier Carrasco. First-Principles Study of Sodium Intercalation in Crystalline $\text{Na}_x\text{Si}_{24}$ ($0 < x < 4$) as Anode Material for Na-ion Batteries. SCIENTIFIC REPORTS. 7, pp. 5350. NATURE PUBLISHING GROUP, 07/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 33** Ting Deng; Wei Zhang; Oier Arcelus; Jin-Gyu Kim; Javier Carrasco; Seung Jo Yoo; Weitao Zheng; Jiafu Wang; Hongwei Tian; Hengbin Zhang; Xiaoqiang Cui; Teofilo Rojo. Atomic-level energy storage mechanism of cobalt hydroxide electrode for pseudocapacitors. NATURE COMMUNICATIONS. 8, pp. 15194. NATURE PUBLISHING GROUP, 05/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 34** Oier Arcelus; Nicolas Suaud; Nebil A. Katcho; Javier Carrasco. Insight from first principles into the stability and magnetism of alkali-metal superoxide nanoclusters. JOURNAL OF CHEMICAL PHYSICS. 146, pp. 184301. AMER INST PHYSICS, 05/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 35** Ariel Lozano; Bruno Escribano; Elena Akhmatkaya; Javier Carrasco. Assessment of van der Waals inclusive density functional theory methods for layered electroactive materials. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 19, pp. 10133 - 10139. Royal Society of Chemistry, 04/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 36** Bruno Escribano; Ariel Lozano; Tijana Radivojevic; Mario Fernandez-Pendas; Javier Carrasco; Elena Akhmatkaya. Enhancing sampling in atomistic simulations of solid-state materials for batteries: a focus on olivine. THEORETICAL CHEMISTRY ACCOUNTS. 136 - 43, Springer, 03/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 37** Lucienne Buannic; Brahim Orayech; Juan-Miguel Lopez Del Amo; Javier Carrasco; Nebil A. Katcho; Frederic Aguesse; William Manalastas; Wei Zhang; John Kilner; Anna Llodes. Dual Substitution Strategy to Enhance Li^+ Ionic Conductivity in $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolyte. CHEMISTRY OF MATERIALS. 29, pp. 1769 - 1778. AMER CHEMICAL SOC, 01/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 38** Nebil A. Katcho; Javier Carrasco; Damien Damien; Elena Gonzalo; Man Han; Frederic Aguesse; Teofilo Rojo. Origins of Bistability and Na Ion Mobility Difference in P_2 - and O_3 - $\text{Na}_2/3\text{Fe}_2/3\text{Mn}_1/3\text{O}_2$ Cathode Polymorphs. ADVANCED ENERGY MATERIALS. 7, pp. 1601477. WILEY-VCH VERLAG GMBH, 01/2017.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 39** Pablo G. Lustemberg; Pedro J. Ramirez; Zongyuan Liu; Ramon A. Gutierrez; David G. Grinter; Javier Carrasco; Sanjaya D. Senanayake; Jose A. Rodriguez; M. Veronica Ganduglia-Pirovano. Room-Temperature Activation of Methane and Dry Re-forming with CO_2 on $\text{Ni-CeO}_2(111)$ Surfaces: Effect of Ce^{3+} Sites and Metal-Support Interactions on C-H Bond Cleavage. ACS CATALYSIS. 6, pp. 8184 - 8191. AMER CHEMICAL SOC, 12/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No



- 40** Benjamin J. Morgan; Javier Carrasco; Gilberto Teobaldi. Variation in Surface Energy and Reduction Drive of a Metal Oxide Lithium-Ion Anode with Stoichiometry: A DFT Study of Lithium Titanate Spinel Surfaces. JOURNAL OF MATERIALS CHEMISTRY A. 4, pp. 17180 - 17192. Royal Society of Chemistry, 10/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 41** Laura Lander; Marine Reynaud; Javier Carrasco; Nebil A. Katcho; Christophe Bellin; Alain Polian; Benoit Baptiste; Gwenaëlle Rousse; Jean-Marie Tarascon. Unveiling the electrochemical mechanisms of $\text{Li}_2\text{Fe}(\text{SO}_4)_2$ polymorphs by neutron diffraction and density functional theory calculations. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 18, pp. 14509 - 14519. Royal Society of Chemistry, 04/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 42** Zongyuan Liu; David Grinter; Pablo Lustemberg; Thuyduong Nguyen-Phan; Erik W. Peterson; Si Luo; Iradwikanari Waluyo; Ethan Crumlin; Dario J Stacchiola; Jing Zhou; Javier Carrasco; H. Fabio Busnengo; M. Veronica Ganduglia-Pirovano; Sanjaya D. Senanayake; Jose A. Rodriguez. Dry Reforming of Methane on a Highly-Active Ni-CeO₂ Catalyst: Effects of Metal-Support Interactions on C-H bond breaking. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION. 55, pp. 7455 - 7459. WILEY-VCH VERLAG GMBH, 03/2016. ISSN 1932-7447
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 43** Amaia Saracibar; Javier Carrasco; Damien Saurel; Montserrat Galceran; Begoña Acebedo; Henri Anne; Mathilde Lepoitevin; Teofilo Rojo; Montse Casas-Cabanas. Investigation of sodium insertion-extraction in the olivine Na_xFePO_4 (0 - x - 1) from first-principles calculations. PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 18, pp. 13045 - 13051. Royal Society of Chemistry, 03/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 44** Imanol Landa-Medrano; Chunmei Li; Nagore Ortiz-Vitoriano; Idoia Ruiz de Larramendi; Javier Carrasco; Teofilo Rojo. Sodium-Oxygen Battery: Steps Toward Reality. JOURNAL OF PHYSICAL CHEMISTRY LETTERS. 7, pp. 1161 - 1166. AMER CHEMICAL SOC, 03/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 45** Vanessa Riffet; Julia Contreras-García; Javier Carrasco; Monica Calatayud. Alkali Ion Incorporation into V₂O₅: A Non-Covalent Interactions Analysis. JOURNAL OF PHYSICAL CHEMISTRY C. 120, pp. 4259 - 4265. AMER CHEMICAL SOC, 02/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 46** Melissa L. Liriano; Javier Carrasco; Emily A. Lewis; Colin J. Murphy; Timothy J. Lawton; Matthew Marcinkowski; Andrew Therrien; Angelos Michaelides; E. Charles H. Sykes. The Interplay of Covalency, Hydrogen Bonding and Dispersion Leads to a Long Range Chiral Network: The Example of 2-Butanol. JOURNAL OF CHEMICAL PHYSICS. 144, pp. 094703. AMER INST PHYSICS, 02/2016.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 47** Lopez-Herrai Maria; Elizabeth Castillo-Martínez; Javier Carretero-Gonzalez; Javier Carrasco; Teofilo Rojo; Michel Armand. Oligomeric-Schiff bases as negative electrodes for sodium ion batteries: unveiling the nature of their active redox centers. ENERGY & ENVIRONMENTAL SCIENCE. 8, pp. 3233 - 3241. ROYAL SOCIETY OF CHEMISTRY, 09/2015.
DOI: 10.1039/C5EE01832C



Type of production: Scientific paper

Format: Journal

Corresponding author: No

- 48** Oier Arcelus; Chunmei Li; Teofilo Rojo; Javier Carrasco. Electronic Structure of Sodium Superoxide Bulk, (100) Surface, and Clusters using Hybrid Density Functional: Relevance for Na₂O₂ Batteries. JOURNAL OF PHYSICAL CHEMISTRY LETTERS. 6, pp. 2027 - 2031. AMER CHEMICAL SOC, 05/2015.

Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

- 49** Javier Carrasco; David Lopez-Duran; Zongyuan Liu; Tomas Duchon; Jaime Evans; Sanjaya D. Senanayake; Ethan J. Crumlin; Vladimir Matolin; Jose A. Rodriguez; M. Veronica Ganduglia-Pirovano. In Situ and Theoretical Studies for the Dissociation of Water on an Active Ni/CeO₂ Catalyst: Importance of Strong Metal-Support Interactions for the Cleavage of O-H Bonds. ANGEWANDTE CHEMIE-INTERNATIONAL EDITION. 54, pp. 3917 - 3921. WILEY-VCH VERLAG GMBH, 03/2015. ISSN 1932-7447

Type of production: Scientific paper

Format: Journal

Corresponding author: No

- 50** Javier Carrasco. Role of van der Waals Forces in Thermodynamics and Kinetics of Layered Transition Metal Oxide Electrodes: Alkali and Alkaline-Earth Ion Insertion into V₂O₅. JOURNAL OF PHYSICAL CHEMISTRY C. 118, pp. 19599 - 19607. AMER CHEMICAL SOC, 08/2014. ISSN 1932-7447

Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

- 51** Delia Fernandez-Torre; Javier Carrasco; Veronica Ganduglia-Pirovano; Ruben Perez. Hydrogen activation, diffusion, and clustering on CeO₂(111): A DFT+U study. JOURNAL OF CHEMICAL PHYSICS. 141, pp. 014703-1 - 014701-9. AMER INST PHYSICS, 07/2014.

Type of production: Scientific paper

Format: Journal

Corresponding author: No

- 52** Colin J. Murphy; Javier Carrasco; Timothy J. Lawton; Melissa L. Liriano; Ashleigh E. Baber.; Emily A. Lewis; Angelos Michaelides; E. Charles H. Sykes. Structure and energetics of hydrogen-bonded networks of methanol on close packed transition metal surfaces. JOURNAL OF CHEMICAL PHYSICS. 141, pp. 014701-1 - 014701-10. AMER INST PHYSICS, 07/2014.

Type of production: Scientific paper

Format: Journal

Corresponding author: No

- 53** Javier Carrasco; Gianvito Vile; Delia Fernandez-Torre; Ruben Perez; Javier Perez-Ramirez; M. Veronica Ganduglia-Pirovano. Molecular-Level Understanding of CeO₂ as a Catalyst for Partial Alkyne Hydrogenation. JOURNAL OF PHYSICAL CHEMISTRY C. 118, pp. 5352 - 5360. AMER CHEMICAL SOC, 03/2014. ISSN 1932-7447

Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

- 54** Javier Carrasco; Wei Liu; Angelos Michaelides; Alexander Tkatchenko. Insight into the description of van der Waals forces for benzene adsorption on transition metal (111) surfaces. JOURNAL OF CHEMICAL PHYSICS. 140, pp. 084704-1 - 084704-10. AMER INST PHYSICS, 02/2014.

Type of production: Scientific paper

Format: Journal

Corresponding author: Yes

- 55** Wei Liu; Sergey N Filimonov; Javier Carrasco; Alexandre Tkatchenko. Molecular switches from benzene derivatives adsorbed on metal surfaces. NATURE COMMUNICATIONS. 4, pp. 2569. NATURE PUBLISHING GROUP, 10/2013.

Type of production: Scientific paper

Format: Journal

Corresponding author: No

- 56** Javier Carrasco; Laura Barrio; Ping Liu; Jose A. Rodriguez; M. Veronica Ganduglia-Pirovano. Theoretical Studies of the Adsorption of CO and C on Ni(111) and Ni/CeO₂(111): Evidence of a Strong Metal-Support Interaction. JOURNAL OF PHYSICAL CHEMISTRY C. 117 - 16, pp. 8241 - 8250. AMER CHEMICAL SOC, 04/2013. ISSN 1932-7447
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 57** Javier Carrasco; Jiri Klimes; Angelos Michaelides. The role of van der Waals forces in water adsorption on metals. JOURNAL OF CHEMICAL PHYSICS. 138 - 2, pp. 024708-1 - 024708-9. AMER INST PHYSICS, 01/2013. ISSN 0021-9606
Type of production: Scientific paper **Format:** Journal
Corresponding author: Yes
- 58** Wei Liu; Javier Carrasco; Biswajit Santra; Angelos Michaelides; Matthias Scheffler; Alexandre Tkatchenko. Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. PHYSICAL REVIEW B. 86 - 24, pp. 245405-1 - 245405-6. AMER PHYSICAL SOC, 12/2012. ISSN 1098-0121
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 59** Javier Carrasco; Andrew Hodgson; Angelos Michaelides. A molecular perspective of water at metal interfaces. NATURE MATERIALS. 11 - 8, pp. 667 - 674. NATURE PUBLISHING GROUP, 08/2012. ISSN 1476-1122
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 60** Delia Fernandez-Torre; Krzysztof Kosmider; Javier Carrasco; M. Veronica Ganduglia-Pirovano; Ruben Perez. Insight into the Adsorption of Water on the Clean CeO₂(111) Surface with van der Waals and Hybrid Density Functionals. JOURNAL OF PHYSICAL CHEMISTRY C. 116 - 25, pp. 13584 - 13593. AMER CHEMICAL SOC, 06/2012. ISSN 1932-7447
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 61** Francesc Vines; Javier Carrasco; Stefan T. Bromley. Nanoscale thermal stabilization via permutational premelting. PHYSICAL REVIEW B. 85 - 19, pp. 195425-1 - 195425-6. AMER PHYSICAL SOC, 05/2012. ISSN 1098-0121
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 62** Timothy J. Lawton; Javier Carrasco; Ashleigh E. Baber; Angelos Michaelides; E. Charles H. Sykes. Hydrogen-bonded assembly of methanol on Cu(111). PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 14 - 33, pp. 11846 - 11852. ROYAL SOC CHEMISTRY, 2012. ISSN 1463-9076
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 63** Matthew Forster; Rasmita Raval; Javier Carrasco; Angelos Michaelides; Andrew Hodgson. Water-hydroxyl phases on an open metal surface: breaking the ice rules. CHEMICAL SCIENCE. 3 - 1, pp. 93 - 102. ROYAL SOC CHEMISTRY, 2012.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 64** Timothy J. Lawton; Javier Carrasco; Ashleigh E. Baber; Angelos Michaelides; E. Charles H. Sykes. Visualization of Hydrogen Bonding and Associated Chirality in Methanol Hexamers. PHYSICAL REVIEW LETTERS. 107 - 25, AMER PHYSICAL SOC, 12/2011. ISSN 0031-9007

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

- 65** Wanda Lew; Matthew C. Crowe; Charles T. Campbell; Javier Carrasco; Angelos Michaelides. The Energy of Hydroxyl Coadsorbed with Water on Pt(111). JOURNAL OF PHYSICAL CHEMISTRY C. 115 - 46, pp. 23008 - 23012. AMER CHEMICAL SOC, 11/2011. ISSN 1932-7447

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 66** Maria Alejandra Florida Addato; Aldo A. Rubert; Guillermo A. Benitez; Mariano H. Fonticelli; Javier Carrasco; Pilar Carro; Roberto C. Salvarezza. Alkanethiol Adsorption on Platinum: Chain Length Effects on the Quality of Self-Assembled Monolayers. JOURNAL OF PHYSICAL CHEMISTRY C. 115 - 36, pp. 17788 - 17798. AMER CHEMICAL SOC, 09/2011. ISSN 1932-7447

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 67** Javier Carrasco; Biswajit Santra; Jiri Klimes; Angelos Michaelides. To Wet or Not to Wet? Dispersion Forces Tip the Balance for Water Ice on Metals. PHYSICAL REVIEW LETTERS. 106 - 2, pp. 026101-1 - 026101-4. AMER PHYSICAL SOC, 01/2011. ISSN 0031-9007

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 68** Matthew Forster; Rasmita Raval; Andrew Hodgson; Javier Carrasco; Angelos Michaelides. c(2 x 2) Water-Hydroxyl Layer on Cu(110): A Wetting Layer Stabilized by Bjerrum Defects. PHYSICAL REVIEW LETTERS. 106 - 4, pp. 046103-1 - 046103-4. AMER PHYSICAL SOC, 01/2011. ISSN 0031-9007

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 69** Xiao Liang Hu; Javier Carrasco; Jiri Klimes; Angelos Michaelides. Trends in water monomer adsorption and dissociation on flat insulating surfaces (vol 13, pg 12447, 2010). PHYSICAL CHEMISTRY CHEMICAL PHYSICS. 13 - 48, pp. 21652 - 21652. ROYAL SOC CHEMISTRY, 2011. ISSN 1463-9076

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 70** Michael Mehlhorn; Javier Carrasco; Angelos Michaelides; Karina Morgenstern. Local Investigation of Femtosecond Laser Induced Dynamics of Water Nanoclusters on Cu(111). PHYSICAL REVIEW LETTERS. 103 - 2, pp. 026101-1 - 026101-4. AMER PHYSICAL SOC, 07/2009. ISSN 0031-9007

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 71** Javier Carrasco; Angelos Michaelides; Matthew Forster; Sam Haq; Rasmita Raval; Andrew Hodgson. A one-dimensional ice structure built from pentagons. NATURE MATERIALS. 8 - 5, pp. 427 - 431. NATURE PUBLISHING GROUP, 05/2009. ISSN 1476-1122

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 72** Javier Carrasco; Angelos Michaelides; Matthias Scheffler. Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. JOURNAL OF CHEMICAL PHYSICS. 130 - 18, pp. 184707-1 - 184707-11. AMER INST PHYSICS, 05/2009. ISSN 0021-9606

Type of production: Scientific paper**Format:** Journal**Corresponding author:** No

- 73** J. Carrasco; F. Illas; N. Lopez. Dynamic ion pairs in the adsorption of isolated water molecules on alkaline-earth oxide (001) surfaces. *Physical Review Letters*. 100, pp. 016101-1 - 016101-4. American Physical Society, 2008.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 74** K. Morgenstern; H. Gawronski; J. Carrasco; A. Michaelides. Manipulation and control of hydrogen bond dynamics in adsorbed ice nanoclusters. *Physical Review Letters*. 101, pp. 136102-1 - 136102-4. American Physical Society, 2008.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 75** C. Loschen; J. Carrasco; K. M. Neyman; F. Illas. First-principles LDA plus U and GGA plus U study of cerium oxides: Dependence on the effective U parameter. *Physical Review B*. 75, pp. 035115-1 - 035115-8. American Physical Society, 2007.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 76** J. Carrasco; F. Illas; S. T. Bromley. Ultra-low-density nanocage-based metal oxide polymorphs. *Physical Review Letters*. 99, pp. 235502-1 - 235502-4. American Physical Society, 2007.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 77** J. Carrasco; N. Lopez; F. Illas; H.-J. Freund. Bulk and surface oxygen vacancy formation and diffusion in single-crystals, ultra-thin films and metal grown oxide structures. *Journal of Chemical Physics*. 125, pp. 074711-1 - 074711-6. American Institute of Physics, 2006.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 78** J. Carrasco; F. Illas; N. Lopez; E. A. Kotomin; Yu. F. Zhukovskii; A. Evarestov; Yu. A. Mastrikov; S. Piskunov; J. Maier. First-principles calculations of the atomic and electronic structure of F centers in the bulk and on the (001) surface of SrTiO₃. *Physical Review B*. 73, pp. 064106-1 - 064106-11. American Physical Society, 2006.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 79** J. Carrasco; C. Sousa; F. Illas; P. V. Sushko; A. L. Shluger. Optical absorption and luminescence energies of F centers in CaO from ab initio embedded cluster calculations. *Journal of Chemical Physics*. 125, pp. 074710-1 - 074710-9. American Institute of Physics, 2006.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 80** L. Giordano; J. Carrasco; C. Di Valentin; F. Illas; G. Pacchioni. Vibrational and EPR properties of free and MgO supported AuCO complexes. *Journal of Chemical Physics*. 124, pp. 174709-1 - 174709-8. American Institute of Physics, 2006.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 81** M. Sterrer; M. Yulikov; T. Risse; H.-J. Freund; J. Carrasco; F. Illas; C. Di Valentin; L. Giordano; G. Pacchioni. When the reporter induces the effect: CO on Au₁/MgO(100)/Mo(100). *Angewandte Chemie International Edition*. 45, pp. 2633 - 2635. Wiley, 2006.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No

- 82** J. Carrasco; F. Illas; N. Lopez; E. A. Kotomin; Yu. F. Zhukovskii; S. Piskunov; J. Maier; K. Hermansson. First principles simulations of F centers in cubic SrTiO₃. *Physica Status Solidi C*. 2, pp. 153 - 158. 2005.
Type of production: Scientific paper **Format:** Journal
- 83** J. Carrasco; N. Lopez; C. Sousa; F. Illas. First-principles study of the optical transitions of F centers in the bulk and on the (0001) surface of alpha-Al₂O₃. *Physical Review B*. 72, pp. 054109-1 - 054109-9. American Physical Society, 2005.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 84** J. Carrasco; N. Lopez; F. Illas. On the convergence of isolated neutral oxygen vacancy and divacancy properties in metal oxides using supercell models. *Journal of Chemical Physics*. 122, pp. 224705-1 - 224705-14. American Institute of Physics, 2005.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 85** J. Carrasco; N. Lopez; F. Illas. First principles analysis of the stability and diffusion of oxygen vacancies in metal oxides. *Physical Review Letters*. 93, pp. 225502-1 - 225502-4. American Physical Society, 2004.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 86** J. Carrasco; J. R. B. Gomes; F. Illas. Theoretical study of bulk and surface oxygen and aluminum vacancies in alpha-Al₂O₃. *Physical Review B*. 69, pp. 064116-1 - 064116-13. American Physical Society, 2004.
Type of production: Scientific paper **Format:** Journal
Corresponding author: No
- 87** Claudio Cazorla; María Verónica Ganduglia-Pirovano; Javier Carrasco. Editorial: The Role of Non-stoichiometry in the Functional Properties of Oxide Materials. *FRONTIERS IN CHEMISTRY*. 7, pp. 547. Frontiers, 08/2019.
Type of production: Scientific edition **Format:** Journal
Corresponding author: No
- 88** Heng Zhang; Fangfang Chen; Javier Carrasco. Nanoscale modelling of polymer electrolytes for rechargeable batteries. *ENERGY STORAGE MATERIALS*. 36, pp. 77 - 90. Elsevier, 04/2021.
Type of production: Review **Format:** Journal
Corresponding author: Yes

Works submitted to national or international conferences

- 1** **Title of the work:** Understanding Li-ion conductivity in garnet-based and composite polymer-ceramic solid electrolytes using atomistic simulations
Name of the conference: XV Spanish National Meeting on Electroceramics
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Vitoria, Basque Country, Spain
Date of event: 07/07/2021
End date: 09/07/2021
Organising entity: SOCIEDAD ESPAÑOLA DE CERAMICA Y VIDRIO
Javier Carrasco; Mauricio Bonilla; Fabián García Daza; Pierre Ranque; Frederic Aguesse; Elena Akhmatskaya.

- 2** **Title of the work:** Nanoscale modelling of polymer electrolytes for solid-state batteries
Name of the conference: 7th International Conference on Mechanical Structures and Smart Materials
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Online,
Date of event: 15/06/2021
End date: 15/06/2021
Organising entity: International Conference on Mechanical Structures and Smart Materials
Javier Carrasco.
- 3** **Title of the work:** Computational exploration of energy storage materials using theoretical chemistry and machine learning
Name of the conference: SIAM Conference of Mathematical Aspects of Materials Science, MS-21
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Online,
Date of event: 17/05/2021
End date: 28/05/2021
Organising entity: Society for Industrial and Applied Mathematics; Basque Center for Applied Mathematics
Javier Carrasco.
- 4** **Title of the work:** Atomistic Modelling of Polymer Electrolytes for Solid-State Batteries
Name of the conference: Computer and Modeling and Simulation, CMS 2021
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Online,
Date of event: 24/03/2021
End date: 24/03/2021
Organising entity: Department of Chemistry, University of Aveiro
Javier Carrasco.
- 5** **Title of the work:** Computational screening of Li and Na fast ion conductors using high-throughput bond-valence calculations, machine-learning analysis and experimental validation
Name of the conference: European perspectives on batteries of the future
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Online,
Date of event: 25/05/2020
End date: 26/05/2020
Organising entity: University of Uppsala - Battery 2030, funded by European Union's Horizon 2020
Montserrat Casas-Cabanas; Javier Carrasco.

- 6** **Title of the work:** Understanding Li-ion transport and conductivity in Ga- and Alsubstituted garnet-type Li La Zr O solid electrolytes using atomistic simulations
Name of the conference: 44th International Conference and Expo on Advanced Ceramics and Composites
Type of event: Conference
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
Corresponding author: Yes
City of event: Daytona Beach, United States of America
Date of event: 26/01/2020
End date: 31/01/2020
Organising entity: The American Ceramic Society
Javier Carrasco; Fabian A. Garcia Daza; Mauricio R. Bonilla; Elena Akhmatskaya.
- 7** **Title of the work:** Computational screening of Li and Na fast ion conductors using high-throughput bond-valence calculations and machine-learning analysis
Name of the conference: TechConnect World Innovation Conference & Expo
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral **Reasons for participation:** Review before communication acceptance
City of event: Boston, United States of America
Date of event: 17/06/2019
End date: 19/06/2019
Organising entity: TechConnect World
J. Carrasco.
- 8** **Title of the work:** Atomistic-level insight into the energy storage properties of layered transition metal oxides
Name of the conference: seminar at Jilin University
Type of event: Seminar
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Changchun, China
Date of event: 16/10/2018
Organising entity: Jilin University
J. Carrasco.
- 9** **Title of the work:** Ion insertion into 2D layered oxide structures for energy storage: A molecular-level perspective using first-principles calculations
Name of the conference: Energy Materials and Nanotechnology Barcelona Meeting 2018
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Barcelona, Catalonia, Spain
Date of event: 12/09/2018
Organising entity: EMN Meetings
J. Carrasco.
- 10** **Title of the work:** Molecular modelling, high performance computing, and the pursuit of better batteries
Name of the conference: 11th RES Users' Conference
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Santiago de Compostela, Galicia, Spain



Date of event: 28/09/2017

Organising entity: Spanish Supercomputing Network

J. Carrasco.

- 11 Title of the work:** Atomistic modelling of materials for rechargeable batteries
Name of the conference: seminar at Ningbo Institute of Materials Technology & Engineering
Type of event: Seminar
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Ningbo, China
Date of event: 25/04/2017
Organising entity: Chinese Academy of Sciences **Type of entity:** Public Research Body
J. Carrasco.

- 12 Title of the work:** Atomistic modelling of materials for rechargeable batteries
Name of the conference: Seminar at the Beijing Computational Science Research Center
Type of event: Seminar
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Beijing, China
Date of event: 18/04/2017
Organising entity: Beijing Computational Science Research Center **Type of entity:** R&D Centre
J. Carrasco.

- 13 Title of the work:** Atomistic modelling studies of electrode materials for rechargeable lithium and sodium batteries
Name of the conference: 10th RES Users' Conference
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Leon, Castile and León, Spain
Date of event: 09/2016
Organising entity: Spanish Supercomputing Network
J. Carrasco.

- 14 Title of the work:** First-principles study of crystal structure and stability of $\text{Li}_2\text{Fe}(\text{NCN})_2$ and $\text{Na}_2\text{Fe}(\text{NCN})_2$
Name of the conference: Gordon Research Conference on Materials Discovery
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster **Reasons for participation:** Review before acceptance
City of event: New London, United States of America
Date of event: 07/2016
Organising entity: Gordon Research Conferences
J. Carrasco; Nebil A. Katcho.

- 15 Title of the work:** Role of Polymorphism in the Electrochemical Behavior of Electrode Materials for Rechargeable Batteries: a First-Principles Perspective
Name of the conference: iPolymorphs: Novel Routes to Inorganic Polymorphs
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication **Reasons for participation:** Review before acceptance



Date of event: 06/2016

City organizing entity: San Sebastian, Basque Country, Spain

J. Carrasco.

- 16 Title of the work:** Ion insertion into layered transition metal oxides for batteries: Insight from van der Waals density functional

Name of the conference: Psi-k 2015 Conference

Type of event: Conference

Geographical area: Non EU International

Type of participation: Participatory - oral communication

Reasons for participation: Review before acceptance

Date of event: 09/2015

City organizing entity: San Sebastian, Basque Country, Spain

J. Carrasco.

- 17 Title of the work:** Advances in treating van der Waals forces in density functional theory: From adsorption of molecules on surfaces to ion insertion in sparse matter

Name of the conference: 4th International Symposium on Ceramics Nanotune Technology

Type of event: Conference

Geographical area: Non EU International

Type of participation: Participatory - invited/keynote talk

Reasons for participation: Upon invitation

Date of event: 03/2015

City organizing entity: Nagoya, Japan

J. Carrasco.

- 18 Title of the work:** Role of van der Waals forces in alkali and alkaline-earth ion insertion into layered transition metal oxide electrodes for batteries

Name of the conference: CECAM/Psi-k Research Conference: Frontiers of First-Principles Simulations: Materials Design and Discovery

Type of event: Conference

Geographical area: European Union

Type of participation: Participatory - poster

Reasons for participation: Review before acceptance

Date of event: 02/2015

City organizing entity: Berlin, Germany

J. Carrasco.

- 19 Title of the work:** The role of van der Waals forces in thermodynamics and kinetics of layered transition metal oxide electrodes: Alkali and alkaline-earth ion insertion into V₂O₅

Name of the conference: 2nd International Union of Materials Research Societies (IUMRS) – International Conference of Young Researchers on Advanced Materials

Type of event: Conference

Geographical area: Non EU International

Type of participation: Participatory - invited/keynote talk

Reasons for participation: Upon invitation

Date of event: 10/2014

City organizing entity: Haikou, China

J. Carrasco.

- 20 Title of the work:** The role of van der Waals forces in thermodynamics and kinetics of layered transition metal oxide electrodes: Alkali and alkaline-earth ion insertion into V₂O₅

Name of the conference: 3rd TYC Energy Materials Workshop: Materials for Electrochemical Energy Storage

Type of event: Workshop

Geographical area: Non EU International

Type of participation: Participatory - poster



Reasons for participation: Review before acceptance

Date of event: 09/2014

City organizing entity: London, United Kingdom

J. Carrasco.

- 21 Title of the work:** First-principles study of Na insertion/extraction in the FePO₄-NaFePO₄ system for cathode material in Na-ion batteries

Name of the conference: Workshop of the CMST COST Action CM1104: Reducible oxide chemistry, structure and functions

Type of event: Workshop

Geographical area: European Union

Type of participation: 'Participatory - poster

Reasons for participation: Review before acceptance

Date of event: 04/2014

City organizing entity: Zaragoza, Spain

J. Carrasco; A. Saracibar.

- 22 Title of the work:** DFT study of acetylene hydrogenation on CeO₂(111)

Name of the conference: Workshop of the CMST COST Action CM1104: Reducible oxide chemistry, structure and functions

Type of event: Workshop

Geographical area: European Union

Type of participation: Participatory - oral communication

Reasons for participation: Review before acceptance

Date of event: 04/2013

City organizing entity: Vienna, Austria

J. Carrasco; M. V. Ganduglia-Pirovano; G. Vile; J. Perez-Ramirez; D. Fernandez-Torre; R. Perez.

- 23 Title of the work:** First-Principles Simulations in Chemical Physics

Name of the conference: Seminar at CIC Energigune

Type of event: Seminar

Type of participation: Participatory - invited/keynote talk

Reasons for participation: Upon invitation

City of event: Miñano, Basque Country, Spain

Date of event: 24/01/2013

Organising entity: CIC Energigune

J. Carrasco.

- 24 Title of the work:** Water-hydroxyl phases on Cu(110): breaking the ice rules

Name of the conference: European Conference on Surface Science (ECOSS 29)

Type of event: Conference

Geographical area: European Union

Type of participation: 'Participatory - poster

Reasons for participation: Review before acceptance

City of event: Edinburgh, United Kingdom

Date of event: 09/2012

J. Carrasco; M. Forster; R. Raval; A. Michaelides; A. Hodgson.

- 25 Title of the work:** Understanding structure and function of Ni-CeO₂ catalysts: A theoretical perspective

Name of the conference: Initial Workshop of the CMST COST Action CM1104: Reducible oxide chemistry, structure and functions

Type of event: Workshop

Geographical area: European Union

Type of participation: 'Participatory - poster

Reasons for participation: Review before acceptance



Date of event: 09/2012

City organizing entity: Prague, Praha, Czech Republic

- 26** **Title of the work:** A molecular perspective of water at metal interfaces
Name of the conference: Seminar at the School of Physics
Type of event: Seminar
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Beijing, China
Date of event: 22/06/2012
Organising entity: Peking University **Type of entity:** University
J. Carrasco.
- 27** **Title of the work:** A molecular perspective of water at metal interfaces
Name of the conference: Seminar at the Beijing Computational Science Research Center
Type of event: Seminar
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Beijing, China
Date of event: 11/06/2012
Organising entity: Beijing Computational Science Research Center **Type of entity:** R&D Centre
J. Carrasco.
- 28** **Title of the work:** Understanding structure and function of Ni-CeO₂ catalysts: A theoretical perspective
Name of the conference: 1st Annual Congress of Advanced Materials
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Beijing, China
Date of event: 06/2012
J. Carrasco; L. Barrio; M. V. Ganduglia-Pirovano.
- 29** **Title of the work:** To wet or not to wet? Dispersion forces tip the balance for water ice on metals
Name of the conference: American Physical Society March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication **Reasons for participation:** Review before acceptance
City of event: Boston, United States of America
Date of event: 03/2012
J. Carrasco; B. Santra; J. Klimes; A. Michaelides.
- 30** **Title of the work:** To wet or not to wet? Dispersion forces tip the balance for water ice on metals
Name of the conference: Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC-2011)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication **Reasons for participation:** Review before acceptance
City of event: Santiago de Compostela, Galicia, Spain
Date of event: 07/2011
J. Carrasco; B. Santra; J. Klimes; A. Michaelides.



- 31 Title of the work:** Insight into water-metal interactions from van der Waals density functional theory
Name of the conference: Theoretical Modeling of Materials (Satellite Meeting of the WATOC-2011)
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster **Reasons for participation:** Open access
City of event: Barcelona, Catalonia, Spain
Date of event: 07/2011
 J. Carrasco; B. Santra; J. Klimes; A. Michaelides.
- 32 Title of the work:** Insight into water-metal interactions from van der Waals density functional theory
Name of the conference: Understanding Structure and Functions of Reducible Oxide Systems: A Challenge for Theory and Experiment (CECAM-ZCAM Workshop)
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster **Reasons for participation:** Open access
City of event: Zaragoza, Aragon, Spain
Date of event: 04/2011
 J. Carrasco; B. Santra; J. Klimes; A. Michaelides.
- 33 Title of the work:** Insight into water-metal interactions from van der Waals density functional theory
Name of the conference: Materials Science International Conference Eastbourne 2011 (Ms ICE XI)
Type of event: Conference **Geographical area:** National
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Eastbourne, Surrey, East and West Sussex, United Kingdom
Date of event: 01/2011
 J. Carrasco; B. Santra; J. Klimes; A. Michaelides.
- 34 Title of the work:** Insight into water-metal interactions from van der Waals density functional theory
Name of the conference: Psi-k Conference
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication **Reasons for participation:** Review before acceptance
City of event: Berlin, Berlin, Germany
Date of event: 10/2010
 J. Carrasco; B. Santra; J. Klimes; A. Michaelides.
- 35 Title of the work:** A one-dimensional ice structure built from pentagons
Name of the conference: American Physical Society March Meeting
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication **Reasons for participation:** Review before acceptance
City of event: Portland, United States of America
Date of event: 03/2010
 J. Carrasco; A. Michaelides.
- 36 Title of the work:** A novel one dimensional ice structure built from pentagons
Name of the conference: 17th Interdisciplinary Surface Science Conference
Type of event: Conference **Geographical area:** Non EU International
Type of participation: Participatory - oral communication **Reasons for participation:** Open access
City of event: Reading, Berkshire, Buckinghamshire and Oxfordshire, United Kingdom



Date of event: 2009

J. Carrasco; A. Michaelides.

- 37 Title of the work:** Density functional theory studies of water-metal interfaces
Name of the conference: COST D-41: Inorganic Oxide Surfaces and Interfaces
Type of event: Workshop **Geographical area:** European Union
Type of participation: 'Participatory - poster **Reasons for participation:** Upon invitation
City of event: London, Inner London, United Kingdom
Date of event: 2009
J. Carrasco; A. Michaelides.

- 38 Title of the work:** Ice on Cu(110): a novel ice structure built from pentagons and more
Name of the conference: Windermere Water Workshop 2009
Type of event: Workshop **Geographical area:** National
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Windermere, Cumbria, United Kingdom
Date of event: 2009
J. Carrasco; A. Michaelides.

- 39 Title of the work:** Insight into ice formation on metal surfaces
Name of the conference: Uncertainty Principle in Theory and Practice
Type of event: Workshop **Geographical area:** National
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Soderstorf, Germany
Date of event: 2009
J. Carrasco; A. Michaelides.

- 40 Title of the work:** Insight into ice growth on metal surfaces: Revising simple water adsorption concepts
Name of the conference: International Workshop on Multiscale Materials Modeling
Type of event: Workshop **Geographical area:** Non EU International
Type of participation: 'Participatory - poster **Reasons for participation:** Open access
City of event: Berlin, Berlin, Germany
Date of event: 2009
J. Carrasco; A. Michaelides.

- 41 Title of the work:** One dimensional ice growth on Cu(110): a novel ice structure built from pentagons
Name of the conference: Seminar at the Quantum Chemistry Group of Humboldt University
Type of event: Seminar
Type of participation: Participatory - invited/keynote **Reasons for participation:** Upon invitation talk
City of event: Berlin, Berlin, Germany
Date of event: 02/10/2008
Organising entity: Humboldt University **Type of entity:** University
J. Carrasco.

- 42 Title of the work:** One dimensional ice growth on Cu(110): insight from density-functional theory
Name of the conference: European Conference on Surface Science (ECOSS 25)
Type of event: Conference **Geographical area:** European Union

Type of participation: Participatory - oral communication

City of event: Liverpool, Merseyside, United Kingdom

Date of event: 09/2008

J. Carrasco; A. Michaelides; M. Scheffler.

Reasons for participation: Review before acceptance

43 Title of the work: Insight into water molecules bonding on 4d metal surfaces

Name of the conference: Deutsche Physikalische Gesellschaft e.V (German Physical Society), Spring Meeting

Type of event: Conference

Type of participation: Participatory - oral communication

City of event: Berlin, Berlin, Germany

Date of event: 03/2008

J. Carrasco; A. Michaelides; M. Scheffler.

Geographical area: European Union

Reasons for participation: Review before acceptance

44 Title of the work: Insight into water molecules bonding on 4d metal surfaces

Name of the conference: American Physical Society March Meeting

Type of event: Conference

Type of participation: Participatory - oral communication

City of event: New Orleans, United States of America

Date of event: 03/2008

J. Carrasco; A. Michaelides; M. Scheffler.

Geographical area: Non EU International

Reasons for participation: Review before acceptance

45 Title of the work: Insight into water molecules bonding on 4d metal surfaces

Name of the conference: Accurate Energetics of Condensed Matter with Quantum Chemistry (CECAM Workshop)

Type of event: Workshop

Type of participation: Participatory - poster

City of event: Lyon, France

Date of event: 2008

J. Carrasco; A. Michaelides; M. Scheffler.

Geographical area: European Union

Reasons for participation: Open access

46 Title of the work: Insight into water molecules bonding on 4d metal surfaces

Name of the conference: International Workshop: New Horizons in Modeling Surface Processes

Type of event: Workshop

Type of participation: Participatory - poster

City of event: London, Inner London, United Kingdom

Date of event: 2008

J. Carrasco; A. Michaelides; M. Scheffler.

Geographical area: Non EU International

Reasons for participation: Open access

47 Title of the work: The nature of the bonding between water and 4d metal surfaces

Name of the conference: Humboldt Foundation Network Meeting

Geographical area: National

Type of participation: Participatory - poster

City of event: Berlin, Berlin, Germany

Date of event: 2008

J. Carrasco.

Reasons for participation: Upon invitation



- 48** **Title of the work:** On the bonding between H₂O and metal surfaces
Name of the conference: Workshop on Electronic Structure Theory at the Water Surface
Type of event: Workshop **Geographical area:** European Union
Type of participation: Participatory - invited/keynote talk **Reasons for participation:** Upon invitation
City of event: Rijeka, Croatia
Date of event: 2007
J. Carrasco; A. Michaelides; M. Scheffler.
- 49** **Title of the work:** Diffusion of surface oxygen vacancies in MgO metal supported ultra-thin films
Name of the conference: Workshop on Supported Metal Clusters
Type of event: Workshop **Geographical area:** European Union
Type of participation: Participatory - oral communication
City of event: Munich, Germany
Date of event: 2006
- 50** **Title of the work:** First principles study of vacancy profiles in oxides: Thin film effects
Name of the conference: European Conference on Surface Science (ECOSS 23)
Type of event: Conference **Geographical area:** European Union
Type of participation: 'Participatory - poster **Reasons for participation:** Open access
City of event: Berlin, Berlin, Germany
Date of event: 2005
J. Carrasco; F. Illas; N. Lopez.
- 51** **Title of the work:** First principles simulations of F centers in cubic SrTiO₃
Name of the conference: 15th Internacional Conference on Defects in Insulating Materials (ICDIM-2004)
Type of event: Conference **Geographical area:** Non EU International
Type of participation: 'Participatory - poster **Reasons for participation:** Open access
City of event: Riga, Latvia
Date of event: 2004
J. Carrasco; F. Illas; N. Lopez; E. A. Kotomin; Yu. F. Zhukovskii; S. Piskunov; J. Maier; K. Hermansson.
- 52** **Title of the work:** Estabilidad y dinámica de vacantes de oxígeno en óxidos metálicos
Name of the conference: XIX Reunió de la Xarxa de Química Teòrica
Type of event: Workshop **Geographical area:** Regional
Type of participation: Participatory - oral communication **Reasons for participation:** Open access
City of event: Girona, Catalonia, Spain
Date of event: 2003
J. Carrasco; N. Lopez; F. Illas.

Other dissemination activities

Title of the work: A molecule's eye view of water
Name of the event: Royal Society Summer Science Exhibition
Type of event: Fairs and exhibitions
City of event: London, Inner London, United Kingdom
Date of event: 25/06/2010
Organising entity: The Royal Society **Type of entity:** -
City organizing entity: London, Inner London, United Kingdom

R&D management and participation in scientific committees

Scientific, technical and/or assessment committees

Committee title: Associate Editor of Frontiers in Physics and Frontiers in Chemistry - Physical Chemistry and Chemical Physics

Affiliation entity: Frontiers

Start date: 01/04/2019

Organization of R&D activities

- 1** **Title of the activity:** 4rd International Forum on Progress and Trends in Battery and Capacitor Technologies - Power out future 2019

Type of activity: International Conference	Geographical area: Non EU International
City of event: Vitoria, Basque Country, Spain	
Convening entity: CIC Energigune	Type of entity: Innovation and Technology Centres
City convening entity: Vitoria, Basque Country, Spain	
Type of participation: Organiser	
Nº assistants: 150	
Start-End date: 02/07/2019 - 05/07/2019	Duration: 4 days
- 2** **Title of the activity:** XXXVIII Reunión del grupo de electroquímica de la Real Sociedad Española de Química

Type of activity: National Conference	Geographical area: National
City of event: Vitoria, Basque Country, Spain	
Convening entity: CIC Energigune	Type of entity: Innovation and Technology Centres
City convening entity: Vitoria, Basque Country, Spain	
Type of participation: Organiser	
Nº assistants: 150	
Start-End date: 05/07/2017 - 07/07/2017	Duration: 3 days
- 3** **Title of the activity:** 3rd International Forum on Progress and Trends in Battery and Capacitor Technologies - Power out future 2017

Type of activity: International Conference	Geographical area: Non EU International
City of event: Vitoria, Basque Country, Spain	
Convening entity: CIC Energigune	Type of entity: Innovation and Technology Centres
City convening entity: Vitoria, Basque Country, Spain	
Type of participation: Organiser	
Nº assistants: 150	
Start-End date: 02/07/2017 - 05/07/2017	Duration: 3 days
- 4** **Title of the activity:** 2nd International Union of Materials Research Societies – International Conference of Young Researchers on Advanced Materials

Type of activity: Co-chair of Symposium on Modeling and Simulation of Functional Materials	Geographical area: Non EU International
City of event: Haikou, China	
Convening entity: International Union of Materials Research Societies	Type of entity: Associations and Groups



Type of participation: Chairman

Nº assistants: 1.000

Start-End date: 24/10/2014 - 29/10/2014

Evaluation and revision of R&D projects and articles

- 1** **Performed tasks:** Review for Science, Science Advances
Entity where activity was carried out: American Association for the Advancement of Science
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2019
- 2** **Name of the activity:** Review of scientific and technological projects submitted to FONCyT
Performed tasks: Review
Entity where activity was carried out: Agencia Nacional de Promoción Científica y Tecnológica
Type of entity: Public Research Body
City of entity: Argentina
Geographical area: Non EU International
Start date: 2014
- 3** **Performed tasks:** Review for Nature Energy, Nature Catalysis, Nature Communications, Scientific Reports
Entity where activity was carried out: Nature Publishing Group and Springer Nature
Type of entity: Publisher
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2014
- 4** **Performed tasks:** Review for Advance Energy Materials, Batteries & Supercaps, ChemPhysChem, International Journal of Quantum Chemistry
Entity where activity was carried out: Wiley
Type of entity: Publisher
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2013
- 5** **Name of the activity:** Review of scientific and technological projects submitted to ANEP
Performed tasks: Review
Entity where activity was carried out: Agencia Nacional de Evaluación y Prospectiva
Type of entity: State agency
City of entity: Spain
Type of activity: Participation in panels
Geographical area: National
Start date: 2011
- 6** **Performed tasks:** Review for Journal of Catalysis, Nano Energy, Physical Chemistry Letters, Computational Materials Science, Applied Catalysis A: General, Journal of Solid State Chemistry, Journal of Physics and Chemistry of Solids
Entity where activity was carried out: Elsevier
Type of entity: Publisher
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2011



- 7** **Performed tasks:** Journal of the American Chemical Society, Chemistry of Materials, Review for Accounts of Chemical Research, The Journal of Physical Chemistry Letters, Nano Letters, ACS Applied Materials & Interfaces, ACS Applied Energy Materials, ACS Applied Polymer Materials, Inorganic Chemistry, The Journal of Physical Chemistry
Entity where activity was carried out: American Chemical Society **Type of entity:** Publisher
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2010
- 8** **Performed tasks:** Review for Physical Chemistry Chemical Physics, Dalton Transactions, RSC Advances
Entity where activity was carried out: Royal Society of Chemistry **Type of entity:** Publisher
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2010
- 9** **Performed tasks:** Review for The Journal of Chemical Physics, APL Materials
Entity where activity was carried out: American Institute of Physics **Type of entity:** Publisher
Type of activity: Review of articles in scientific or technological journals
Geographical area: Non EU International
Start date: 2010

Other achievements

Stays in public or private R&D centres

- 1** **Entity:** Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
Faculty, institute or centre: Instituto de Catálisis y Petroleoquímica
City of entity: Madrid, Community of Madrid, Spain
Start-End date: 03/2011 - 08/2013 **Duration:** 2 years - 5 months
Goals of the stay: Contracted
Provable tasks: Towards a first principles design of nanocatalytic systems for energy production
- 2** **Entity:** University College London **Type of entity:** University
Faculty, institute or centre: London Centre for Nanotechnology and Department of Chemistry
City of entity: London, Inner London, United Kingdom
Start-End date: 02/2009 - 02/2011 **Duration:** 2 years
Goals of the stay: Post-doctoral
Provable tasks: Towards a first principles understanding of heterogeneous ice nucleation on the nanoscale
- 3** **Entity:** Max Planck Society **Type of entity:** State agency
Faculty, institute or centre: Fritz Haber Institute
City of entity: Berlin, Berlin, Germany
Start-End date: 01/2007 - 01/2009 **Duration:** 2 years
Goals of the stay: Post-doctoral



Provable tasks: Benchmarking the accuracy of density functional theory for treating water-metal and water-water bonding

- 4** **Entity:** Università di Milano-Bicocca **Type of entity:** University
Faculty, institute or centre: Dipartimento di Scienza dei Materiali
City of entity: Milan, Lombardia, Italy
Start-End date: 09/2005 - 12/2005 **Duration:** 3 months
Goals of the stay: Doctorate
Provable tasks: Vibrational properties of AuCO complexes supported on magnesium oxide
- 5** **Entity:** University College London **Type of entity:** University
Faculty, institute or centre: Department of Physics and Astronomy
City of entity: London, Inner London, United Kingdom
Start-End date: 06/2004 - 09/2004 **Duration:** 3 months
Goals of the stay: Doctorate
Provable tasks: Ab initio study of the optical adsorption and luminescence of colour centres in calcium oxide

Obtained grants and scholarships

- 1** **Name of the grant:** Ramon y Cajal fellowship
Aims: Tenure-track
Awarding entity: Ministerio de Ciencia e Innovación. **Type of entity:** - Investigación
Conferral date: 03/2011 **Duration:** 5 years
End date: 02/2016
- 2** **Name of the grant:** Newton International fellowship
Aims: Post-doctoral
Awarding entity: The Royal Society **Type of entity:** Sociedad
Conferral date: 02/2009 **Duration:** 2 years
End date: 01/2011
- 3** **Name of the grant:** Alexander von Humboldt fellowship
Aims: Post-doctoral
Awarding entity: Alexander von Humboldt Foundation **Type of entity:** Foundation
Conferral date: 03/2007 **Duration:** 1 year - 4 months
End date: 07/2008
- 4** **Name of the grant:** Formacion de Profesorado Universitario
Aims: Pre-doctoral
Awarding entity: Ministerio de Ciencia e Innovación. **Type of entity:** - Investigación
Conferral date: 01/2003 **Duration:** 4 years
End date: 12/2006



Scientific societies and professional associations

- 1** **Name of the society:** European Materials Modelling Council
Affiliation entity: European Union's Horizon 2020 **Type of entity:** Public Research Body
City affiliation entity: Brussels, Belgium
Start date: 2019
- 2** **Name of the society:** Regular member
Affiliation entity: American Physical Society
City affiliation entity: Washington, United States of America
Start date: 01/2009

Prizes, mentions and distinctions

Description: 2017 Top 10 Breakthrough of the Year in Electronic Science and Technology of China for the paper "Atomic-level energy storage mechanism of cobalt hydroxide electrode for pseudocapacitors" published in Nature Communications

Awarding entity: Journal of Electronic Science and Technology **Type of entity:** Publisher

City awarding entity: China

Conferral date: 05/2018