



Ion Errea

27 May 1984 Donostia/San Sebastián, Basque Country, Spain

*Condensed Matter Physicists
at the University of the Basque Country*

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Google Scholar scholar.google.es

Education

- 2007–2011 **PhD in Condensed Matter Physics**, *University of the Basque Country (UPV/EHU) and Donostia International Physics Center (DIPC)*, Basque Country, Spain.
- 2002–2007 **Graduated in Physics**, *University of the Basque Country (UPV/EHU)*, Basque Country, Spain.
- 2006–2007 **Erasmus Student**, *University of Groningen*, Netherlands.

Current Positions

- 2018–Present **Research Associate**, *Centro de Física de Materiales (CFM, CSIC-UPV/EHU)*, Donostia/San Sebastián, Basque Country, Spain.
- 2015–Present **Assistant Professor**, *Department of Applied Physics 1, University of the Basque Country (UPV/EHU)*, Donostia/San Sebastián, Basque Country, Spain.
- 2015–Present **Research Associate**, *Donostia International Physics Center (DIPC)*, Donostia/San Sebastián, Basque Country, Spain.

Previous Positions

- 2014–2015 **Post-Doctoral researcher**, *Donostia International Physics Center*, Donostia/San Sebastián, Basque Country, Spain .
 - Anharmonic effects in solids
- 2012–2013 **Post-Doctoral researcher**, *Institut de Minéralogie et de Physique de Milieux Condensés (IMPMC), Université Pierre et Marie Curie (UPMC)*, Paris, France .
 - Development of the Stochastic Self-Consistent Harmonic Approximation.
 - Working at the *Quantum Theory of Materials* group led by Francesco Mauri.

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- 2007–2011 **Pre-Doctoral researcher**, *University of the Basque Country (UPV/EHU) and Donostia International Physics Center (DIPC)*, Basque Country, Spain.
- First-principles calculations of electronic excitations, dynamical properties and superconductivity of solids under high-pressure.
 - Supervised by Aitor Bergara and Vyacheslav Silkin.

Awards and Obtained Grants

- 2016 Selected by the Editorial Board of Journal of Physics: Condensed Matter as an **Emerging Leader**
- 2015 **Finalist of the 2015 Volker Heine Young Investigator Award**
- 2015 *Juan de la Cierva incorporación post-doctoral fellowship* of the **Spanish Ministry of Economy and Competitiveness** (rejected)
- 2012–2014 **Post-doctoral fellowship** of the Department of Education, Universities and Research of the **Basque Government**
- 2008–2011 **Pre-doctoral fellowship** of the Department of Education, Universities and Research of the **Basque Government**
- 2007 Prize for the **best graduate curriculum** in Physics at the University of the Basque Country
- 2006 Erasmus grant
- 2002 High-school finished with honors

Funded Research Projects

As Principal Investigator

- 01/02/2019–31/01/2024 ***Discovery and Characterization of Hydrogen-Based High-Temperature Superconductors.***
- Funding Agency: European Research Council, Starting Grant
 - Principal Investigator: Ion Errea
 - Funding: 1,432,500 €
- 01/03/2019–30/06/2019 ***Quantum Effects on Superconducting Hydrides.***
- Funding Agency: Red Española de Supercomputación, Spain
 - Principal Investigator: Ion Errea
 - Funding: 5,400,000 CPU hours
- 01/07/2017–31/10/2017 ***Phase Transitions and Thermal Conductivity of Thermoelectric SnSe.***
- Funding Agency: Red Española de Supercomputación, Spain
 - Principal Investigator: Ion Errea
 - Funding: 640,000 CPU hours

As member of the work team

- 01/04/2018–31/03/2019 ***Exact Exchange effects on anharmonic vibrational spectra.***
- Funding Agency: PRACE - Partnership for Advanced Computing in Europe
 - Principal Investigator: Matteo Calandra
 - Funding: 17,000,000 CPU hours

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- 2017–2019 ***Excitaciones electrónicas en superficies y nanoestructuras.***
- Funding Agency: Ministerio de Economía y Competitividad, Spain
 - Principal Investigator: Andrés Ayuela
 - Funding: 125,000 €
- 14/03/2016–
14/03/2016 ***High pressure structural, optical and superconducting properties of hydrides.***
- Funding Agency: PRACE - Partnership for Advanced Computing in Europe
 - Principal Investigator: Matteo Calandra
 - Funding: 9,000,000 CPU hours
- 01/09/2014–
31/08/2015 ***Anharmonic Effects in Superconductors, Ferroelectrics, and Thermo-electrics.***
- Funding Agency: PRACE - Partnership for Advanced Computing in Europe
 - Principal Investigator: Matteo Calandra
 - Funding: 9,000,000 CPU hours
- 2014–2016 ***Reactividad, propiedades electrónicas y estructurales de sistemas complejos.***
- Funding Agency: Ministerio de Economía y Competitividad, Spain
 - Principal Investigator: Joseba Iñaki Juaristi Oñiden
 - Funding: 125,000 €
- 2013 ***Propriétés électronique et vibrationnelles des solides.***
- Funding Agency: Grand Equipment National de Calcul Intensif (GENCI), France
 - Principal Investigator: Matteo Calandra
 - Funding: 460,000 CPU hours
- 2011–2013 ***Dinámica electrónica, transporte, plasmónica y microscopía electrónica.***
- Funding Agency: Ministerio de Ciencia e Innovación, Spain
 - Principal Investigator: Andrés Arnau
 - Funding: 229,900 €

Lecturing and Supervision of Students

Postdoctoral Researchers Supervision

- 2019–Present **Supervisor of Raffaello Bianco**, *Centro de Física de Materiales (CSIC-UPV/EHU)*, Basque Country, Spain.
- Topic: *A new first-principles method to calculate the electron-phonon interaction*
 - Supervisors: Ion Errea

PhD Thesis Supervision

- 2019–Present **Supervisor of Francesco Belli's PhD Thesis**, *Centro de Física de Materiales (CSIC-UPV/EHU)*, Basque Country, Spain.
- Title: *A first-principles characterization of superconducting hydrogen compounds with full inclusion of ionic quantum effects*
 - Supervisors: Ion Errea
- 2019–Present **Supervisor of Antonella Meninno's PhD Thesis**, *Centro de Física de Materiales (CSIC-UPV/EHU)*, Basque Country, Spain.
- Title: *A first-principles study of the possibility of high-temperature superconductivity on hydrogen compounds at ambient pressure*
 - Supervisors: Ion Errea

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2017–Present **Supervisor of Donaldi Mancelli's PhD Thesis**, *Donostia International Physics Center, in cotutelle with the University of Bordeaux*, Basque Country, Spain and Bordeaux, France.

- Title: *Matter at Very High Pressures Created by Laser Driven Shock Waves*
- Supervisors: Ion Errea and Dimitri Batani

2016–Present **Supervisor of Unai Aseginolaza's PhD Thesis**, *Centro de Física de Materiales (CSIC-UPV/EHU)*, Basque Country, Spain.

- Title: *Anharmonic effects in thermoelectric materials*
- Supervisors: Ion Errea and Aitor Bergara

2015–2018 **Supervisor of Miguel Borinaga's PhD Thesis**, *Centro de Física de Materiales (CSIC-UPV/EHU)*, Basque Country, Spain.

- Title: *Hydrogen and lithium under high pressure: Superconductivity and other emerging properties*
- Supervisors: Ion Errea and Aitor Bergara
- Grade: *Sobresaliente Cum Laude*

Master Thesis Supervision

2015–2016 **Supervisor of Unai Aseginolaza's Master Thesis**, *Centro de Física de Materiales CSIC-UPV/EHU*, Basque Country, Spain.

- Title: *Anharmonic renormalization of flexural acoustic modes in graphene*
- Supervisors: Ion Errea and Aitor Bergara

2013–2014 **Supervisor of Miguel Borinaga's Master Thesis**, *Centro de Física de Materiales CSIC-UPV/EHU*, Basque Country, Spain.

- Title: *Anharmonic Effects in the High-Pressure Phases of Hydrogen*
- Supervisors: Ion Errea and Aitor Bergara

Bachelor Thesis Supervision

2014–2015 **Supervisor of Unai Aseginolaza's Bachelor Thesis**, *University of the Basque Country (UPV/EHU)*, Basque Country, Spain.

- Title: *Isotope effect in superconducting lithium at high pressure*
- Supervisors: Ion Errea and Aitor Bergara

2013–2014 **Supervisor of Patricia Riego's Bachelor Thesis**, *University of the Basque Country (UPV/EHU)*, Basque Country, Spain.

- Title: *Efectos Anarmónicos en la Superconductividad del Hidrógeno Metálico*
- Supervisors: Ion Errea, Aritz Leonardo, and Aitor Bergara

Lecturing Experience

2018–2019 **Lecturer of "Fundamentos Físicos de la Ingeniería"**, *Gipuzkoako Ingeniaritza Eskola*, University of the Basque Country (UPV/EHU).

2017–2018 **Lecturer of "Fundamentos Físicos de la Ingeniería"**, *Gipuzkoako Ingeniaritza Eskola*, University of the Basque Country (UPV/EHU).

2017–2018 **Lecturer of "Ingeniaritzaren Oinarri Fisikoak"**, *Bilboko Ingeniaritza Eskola*, University of the Basque Country (UPV/EHU).

2016–2017 **Lecturer of "Ingeniaritzaren Oinarri Fisikoak"**, *Bilboko Ingeniaritza Eskola*, University of the Basque Country (UPV/EHU).

2015–2016 **Lecturer of "Ingeniaritzaren Oinarri Fisikoak"**, *Bilboko Ingeniaritza Eskola*, University of the Basque Country (UPV/EHU).

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2011 **Lecturing collaboration in the subject "Teknika Esperimentalak I"**, University of the Basque Country (UPV/EHU).

Research Stays

01/05/2014–31/05/2014 **Institut de Minéralogie et de Physique de Milieux Condensés (IMPMP), Université Pierre et Marie Curie (UPMC), Paris, France.**

- Working with Francesco Mauri and Matteo Calandra
- Topic: "The stochastic self-consistent harmonic approximation"

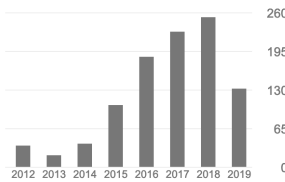
01/09/2010–31/11/2010 **Institut de Minéralogie et de Physique de Milieux Condensés (IMPMP), Université Pierre et Marie Curie (UPMC), Paris, France.**

- Working with Francesco Mauri and Matteo Calandra
- Topic: "The Inverse Isotope Effect in Palladium Hydrides"

Scientific Publications

Summary

- A total of 33 scientific papers, 13 of them as first author and 3 as last author, including 1 Nature, 1 PNAS, 1 Nano Letters, and 5 PRL
- Total number of citations as of 13/05/2019 is 1034 according to Google Scholar
- The h-index as of 13/05/2019 is 14 according to Google Scholar
- Citations evolution according to Google Scholar



Scientific Papers

- 33 "Quantum Enhancement of Charge Density Wave in NbS_2 in the Two-Dimensional Limit",
Raffaello Bianco, Ion Errea, Lorenzo Monacelli, Matteo Calandra, and Francesco Mauri,
Nano Letters 19, 3098 (2019)
- 32 "Phonon collapse and second-order phase transition in thermoelectric $SnSe$ ",
Unai Aseginolaza, Raffaello Bianco, Lorenzo Monacelli, Lorenzo Paulatto, Matteo Calandra, Francesco Mauri, Aitor Bergara, and Ion Errea,
Physical Review Letters 122, 075901 (2019)
- 31 "Ab initio study of the LiH phase diagram at extreme pressures and temperatures",
Sananda Biswas, Ion Errea, Matteo Calandra, Francesco Mauri, and Sandro Scandolo,
Physical Review B 99, 024108 (2019)

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- 30 "Pressure and stress tensor of complex anharmonic crystals within the stochastic self-consistent harmonic approximation ",
Lorenzo Monacelli, Ion Errea, Matteo Calandra, and Francesco Mauri,
Physical Review B 98, 024106 (2018)
- 29 "High-pressure phase diagram of hydrogen and deuterium sulfides from first principles: structural and vibrational properties including quantum and anharmonic effects",
Raffaello Bianco, Ion Errea, Matteo Calandra, and Francesco Mauri,
Physical Review B 97, 214101 (2018)
- 28 "Strong Electron-Phonon and Band Structure Effects in the Optical Properties of High Pressure Metallic Hydrogen",
Miguel Borinaga, Julen Ibañez-Azpiroz, Aitor Bergara, and Ion Errea,
Physical Review Letters 120, 057402 (2018)
- 27 "Strong anharmonicity in the phonon spectra of PbTe and SnTe from first principles",
Guilherme A. S. Ribeiro, Lorenzo Paulatto, Raffaello Bianco, Ion Errea, Francesco Mauri, and Matteo Calandra,
Physical Review B 97, 014306 (2018)
- 26 "Anharmonicity and the isotope effect in superconducting lithium at high pressures: A first-principles approach",
Miguel Borinaga, Unai Aseginolaza, Ion Errea, Matteo Calandra, Francesco Mauri, and Aitor Bergara,
Physical Review B 96, 184505 (2017)
- 25 "Second-order structural phase transitions, free energy curvature, and temperature-dependent anharmonic phonons in the self-consistent harmonic approximation: Theory and stochastic implementation",
Raffaello Bianco, Ion Errea, Lorenzo Paulatto, Matteo Calandra, and Francesco Mauri,
Physical Review B 96, 014111 (2017)
- 24 "Dynamical stability of face centered cubic lithium at 25 GPa",
Miguel Borinaga, Unai Aseginolaza, Ion Errea, and Aitor Bergara,
JJAP Conf. Proc. 6, 011103 (2017)
- 23 "Temperature dependence of X-ray absorption and nuclear magnetic resonance spectra: probing quantum vibrations of light elements in oxides",
Ruidy Nemausat, Christel Gervais, Christian Brouder, Nicolas Trcera, Amélie Bordage, Cristina Coelho-Diogo, Pierre Florian, Aydar Rakhmatullin, Ion Errea, Lorenzo Paulatto, Michele Lazzeri, and Delphine Cabaret,
Physical Chemistry Chemical Physics 19, 6246 (2017)
- 22 "Approaching the strongly anharmonic limit with ab initio calculations of materials' vibrational properties - a colloquium",
Ion Errea,
European Physical Journal B 89, 237 (2016)

- 21 "Anharmonic enhancement of superconductivity in metallic molecular $Cmca - 4$ hydrogen at high pressure: a first-principles study",
Miguel Borinaga, P. Riego, A. Leonardo, Matteo Calandra, Francesco Mauri, Aitor Bergara, and Ion Errea
Journal of Physics: Condensed Matter 28, 494001 (2016)
- 20 "Anharmonic effects in atomic hydrogen: Superconductivity and lattice dynamical stability",
Miguel Borinaga, Ion Errea, Matteo Calandra, Francesco Mauri, and Aitor Bergara,
Physical Review B 93, 174308 (2016)
- 19 "Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system",
Ion Errea, Matteo Calandra, Chris J. Pickard, Joseph R. Nelson, Richard J. Needs, Yinwei Li, Hanyu Liu, Yunwei Zhang, Yanming Ma, and Francesco Mauri,
Nature 532, 81 (2016)
- 18 "Dissociation products and structures of solid H_2S at strong compression",
Yinwei Li, Lin Wang, Hanyu Liu, Yunwei Zhang, Jian Hao, Chris J. Pickard, Joseph R. Nelson, Richard J. Needs, Wentao Li, Yanwei Huang, Ion Errea, Matteo Calandra, Francesco Mauri, and Yanming Ma,
Physical Review B 93, 020103(R) (2016)
- 17 "Phonon effects on x-ray absorption and nuclear magnetic resonances spectroscopies",
Ruidy Nemausat, Delphine Cabaret, Christel Gervais, Christian Brouder, Nicolas Trcera, Amélie Bordage, Ion Errea, and Francesco Mauri,
Physical Review B 92, 144310 (2015)
- 16 "Strong anharmonicity induces quantum melting of charge density wave in $2H-NbSe_2$ under pressure",
Maxime Leroux, Ion Errea, Mathieu Le Tacon, Sophia Michaela Souliou, Gaston Garbarino, Laurent Cario, Alexey Bosak, Francesco Mauri, Matteo Calandra, and Pierre Rodière,
Physical Review B 92, 140303(R) (2015)
- 15 "Hydrogen sulphide at high pressure: a strongly-anharmonic phonon-mediated superconductor",
Ion Errea, Matteo Calandra, Chris J. Pickard, Joseph Nelson, Richard J. Needs, Yinwei Li, Hanyu Liu, Yanming Ma, and Francesco Mauri,
Physical Review Letters 114, 157004 (2015)
- 14 "First-principles calculations of phonon frequencies, lifetimes, and spectral functions from weak to strong anharmonicity: The example of palladium hydrides",
Lorenzo Paulatto, Ion Errea, Matteo Calandra, and Francesco Mauri,
Physical Review B 91, 054304 (2015)
- 13 "Huge anharmonic effects in superconducting hydrides and transition metal dichalcogenides",
Ion Errea, Matteo Calandra, and Francesco Mauri,
Physica Status Solidi (b) 251, 2556 (2014)

- 12 *"Novel superconducting skutterudite-type phosphorus nitride at high pressure from first-principles calculations"*,
Zamaan Raza, Ion Errea, Artem R. Oganov, and A. Marco Saitta,
Scientific Reports 4, 5889 (2014)
- 11 *"Anharmonic free energies and phonon dispersions from the stochastic self-consistent harmonic approximation: Application to platinum and palladium hydrides"*,
Ion Errea, Matteo Calandra, and Francesco Mauri,
Physical Review B 89, 064302 (2014)
- 10 *"First-Principles Theory of Anharmonicity and the Inverse Isotope Effect in Superconducting Palladium-Hydride Compounds"*,
Ion Errea, Matteo Calandra, and Francesco Mauri,
Physical Review Letters 111, 177002 (2013)
- 9 *"Optical properties of calcium under pressure from first-principles calculations"*,
Ion Errea, Bruno Rousseau, Asier Eiguren, and Aitor Bergara,
Physical Review B 86, 085106 (2012)
- 8 *"Enhanced Anharmonicity Under Pressure"*,
Ion Errea, Bruno Rousseau, and Aitor Bergara,
Journal of Physics: Conference Series 377, 012060 (2012)
- 7 *"Isotope effect in the superconducting high-pressure simple cubic phase of calcium from first principles"*,
Ion Errea, Bruno Rousseau, and Aitor Bergara,
Journal of Applied Physics 111, 112604 (2012)
- 6 *"Anharmonic Stabilization of the High-Pressure Simple Cubic Phase of Calcium"*,
Ion Errea, Bruno Rousseau, and Aitor Bergara,
Physical Review Letters 106, 165501 (2011)
- 5 *"Kohn anomalies and enhanced superconductivity in simple systems under pressure: Insights from the nearly free electron model"*,
Bruno Rousseau, Ion Errea, and Aitor Bergara,
Journal of Physics and Chemistry of Solids 71, 1159 (2010)
- 4 *"Electronic collective excitations in compressed lithium from ab initio calculations: importance and anisotropy of local field effects at large momenta"*,
Ion Errea, A. Rodriguez-Prieto, Bruno Rousseau, V. M. Silkin, and Aitor Bergara,
Physical Review B 81, 205105 (2010)
- 3 *"Exotic behavior and new crystal structures of calcium under pressure"*,
Artem R. Oganov, Ying Xu, Yanming Ma, Ion Errea, Aitor Bergara, and Andriy O. Lyakhov,
Proceedings of the National Academy of Sciences 107, 7646 (2010)
- 2 *"Ab Initio Study of Superconducting Hexagonal Be₂Li Under Pressure"*,
Ion Errea, Miguel Martínez-Canales, and Aitor Bergara,
Physical Review B 78, 172501 (2008)

- 1 "*Fermi Surface Nesting and Phonon Instabilities in Simple Cubic Calcium*",
Ion Errea, Miguel Martínez-Canales, and Aitor Bergara,
High Pressure Research 28, 443 (2008)

PhD thesis

- 1 "*Presioak elementu eta aleazio sinpleetan induzitutako konplexutasunaren azterketa lehen-printzipioetan oinarritutako kalkuluen bidez*",
Ion Errea,
UEU (2012),
ISBN: 978-84-8438-401-4

Science popularization publications

- 3 "*Unveiling the origin of the record superconductivity*",
Ion Errea,
Mapping Ignorance 29/04/2015
- 2 "*Harvesting heat to create electricity: A new world record*",
Ion Errea,
Mapping Ignorance 19/11/2014
- 1 "*Isotope Anomalies in Superconductors and the Pairing Mechanism*",
Ion Errea,
Mapping Ignorance 27/06/2014

Contributions to International Conferences and Workshops as Presenting Author

Invited Lectures

- 16 **Joint Workshop between MOLSPIN and NANOCOBYBRI: Superconductivity meets Molecular Spins**, *Lisboa, Portugal, 20/03/2019-22/03/2019*,
"*Near room temperature superconductivity in hydrides*".
[Ion Errea](#)
- 15 **International Symposium: Superconductivity and Pressure: A Fruitful Relationship on the Road to Room Temperature Superconductivity**, *Madrid, Spain, 21/05/2018-22/05/2018*,
"*Ab Initio Calculations on Superconducting Hydrides: Superconductivity and Optical Properties in H₃S and Hydrogen*".
[Ion Errea](#)
- 14 **APS March Meeting 2018**, *Los Angeles, USA, 05/03/2018-09/03/2018*,
"*Anharmonic Properties of Solids within the Stochastic Self-Consistent Harmonic Approximation: Phonons, Second-Order Structural Phase Transitions, and Thermal Properties*".
[Ion Errea](#)

- 13 **Anharmonicity and Thermal Properties of Solids**, *Paris, France*, 10/01/2018-12/01/2018,
"Anharmonic Properties of Solids within the Stochastic Self-Consistent Harmonic Approximation: Phonons, Second-Order Structural Phase Transitions, and Thermal Properties."
[Ion Errea](#)
- 12 **European High Pressure Research Group Meeting**, *Poznan, Poland*, 03/09/2017-08/09/2017,
"Phase Transitions from First-Principles: Quantum Symmetrization of Hydrogen Bonds in H₃S".
[Ion Errea](#)
- 11 **Shanghai International Crystallographic School working with Bilbao Crystallographic Server**, *Shanghai, China*, 11/06/2017-17/06/2017,
"Phonons in Solids: Theory and DFT Approaches" and *"Computer Laboratory: BCS (and Quantum Espresso) at Play in Phonon Calculations"*.
[Ion Errea](#)
- 10 **Materialen Zientzia eta Teknologia III. kongresua**, *Markina, Basque Country, Spain*, 05/07/2016-06/07/2016,
"Simulazio kuantikoak: materialen propietateak oinarritzko osagaietatik abiatuta".
[Ion Errea](#)
- 9 **10th congress on Electronic Structure: Principles and Applications (ESPA2016)**, *Castellón de la Plana, Spain*, 28/06/2016-01/07/2016,
"Quantum hydrogen-bond symmetrization and high-temperature superconductivity in the hydrogen sulfide system".
[Ion Errea](#)
- 8 **iPolymorphs: Novel Routes to Inorganic Polymorphs**, *Donostia/San Sebastián, Basque Country, Spain*, 22/06/2016-24/06/2016,
"Record superconductivity in the sulfur hydride system".
[Ion Errea](#)
- 7 **International Workshop SUPERHYDRIDES**, *Rome, Italy*, 09/05/2016-10/05/2016,
"Quantum Motion and Anharmonicity in Superconducting Hydrides".
[Ion Errea](#)
- 6 **Psi-K 2015 Conference**, *Donostia/San Sebastián, Basque Country, Spain*, 06/09/2015-10/09/2015,
"Efficient Ab Initio Calculation of Anharmonic Properties in Solids".
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 5 **Workshop MANA-DIPC "Nanostructures and Complex Functional Materials"**, *Donostia/San Sebastián, Basque Country, Spain*, 27/08/2015-28/08/2015,
"Vibrational and superconducting properties of transition metal dichalcogenides from first-principles".
[Ion Errea](#), Matteo Calandra, and Francesco Mauri

- 4 **IUMRS-ICYRAM 2014 Second International Conference of Young Researchers on Advanced Materials**, *Haikou, China*, 24/10/2014-27/10/2014, *"Calculating vibrational properties in strongly anharmonic systems"*.
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 3 **26th Annual Workshop on Recent Developments in Electronic Structure Theory**, *University of North Texas Denton, USA*, 18/05/2014-21/05/2014, *"Anharmonic effects in superconductors, metallic hydrides, and layered materials from the stochastic self-consistent harmonic approximation"*.
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 2 **28th International Winterschool on Electronic Properties of Novel Materials**, *Kirchberg in Tirol, Austria*, 08/03/2014-15/03/2014, *"Anharmonic effects in superconductors, metallic hydrides, and layered materials"*.
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 1 **International workshop on computational physics and materials science ("Total energy and force methods")**, *Lausanne, Switzerland*, 09/01/2014-11/01/2014, *"Anharmonic Effects from the Stochastic Self-Consistent Harmonic Approximation: The Inverse Isotope Effect in Palladium Hydrides"*.
[Ion Errea](#), Matteo Calandra, and Francesco Mauri

Oral Contributions

- 6 **Graphene Week 2018**, *Donostia/San Sebastián, Basque Country, Spain*, 10/09/2018-14/09/2018, *"CDW temperature in bulk and monolayer transition metal dichalcogenides from first-principles"*.
[Ion Errea](#), Raffaello Bianco, Matteo Calandra, and Francesco Mauri
- 5 **International conference on Novel 2D materials explored via scanning probe microscopy and spectroscopy**, *Donostia/San Sebastián, Basque Country, Spain*, 25/06/2018-29/06/2018, *"CDW temperature in bulk and monolayer transition metal dichalcogenides from first-principles"*.
[Ion Errea](#), Raffaello Bianco, Matteo Calandra, and Francesco Mauri
- 4 **Joint AIRAPT-25 and EHPRG-53 "International Conference on High Pressure Science and Technology"**, *Madrid, Spain*, 30/08/2015-04/09/2015, *"Hydrogen Sulfide at High Pressure: a Strongly Anharmonic Phonon Mediated Superconductor"*.
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 3 **15th International Conference on Vibrations at Surfaces**, *Donostia/San Sebastián, Basque Country, Spain*, 22/06/2015-26/06/2015, *"First-Principles Calculation of Strongly Anharmonic Phonons in Transition Metal Dichalcogenides: The Example of NbSe₂"*.
[Ion Errea](#), Matteo Calandra, and Francesco Mauri

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- 2 **51st EHPRG International Meeting**, London, UK, 01/09/2013-06/09/2013,
"Anharmonic effects in superconducting hydrides and simple elements under pressure from the self-consistent harmonic approximation".
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 1 **46th EHPRG International Conference**, Valencia, Spain, 07/09/2008-12/09/2008,
"Superconducting Hexagonal Be₂Li Under Pressure".
[Ion Errea](#), Miguel Martínez-Canales, and Aitor Bergara

Poster Contributions

- 11 **XVII International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, Trieste, Italy, 09/01/2019-11/09/2019,
"CDW temperature in bulk and monolayer transition metal dichalcogenides from first-principles".
[Ion Errea](#), Raffaello Bianco, Lorenzo Monacelli, Matteo Calandra, and Francesco Mauri
- 10 **Interaction Effects in Graphene and Related Materials**, Donostia/San Sebastián, Basque Country, Spain, 13/07/2015-17/07/2015,
"Calculating Strongly Anharmonic Phonons in Transition Metal Dichalcogenides".
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 9 **Electron-vibration coupling: theoretical and numerical challenges**, Lausanne, Switzerland, 27/05/2015-29/05/2015,
"Efficient ab initio calculation of anharmonic properties in solids: the stochastic self-consistent harmonic approximation".
[Ion Errea](#), Lorenzo Paulatto, Matteo Calandra, and Francesco Mauri
- 8 **XVII International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, Trieste, Italy, 15/01/2015-17/01/2015,
"Efficient ab initio calculation of anharmonic properties in solids: the stochastic self-consistent harmonic approximation".
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 7 **Réunion générale du GDR CORREL**, Paris, France, 27/11/2013-29/11/2013,
"Anharmonic free energies and vibrational frequencies from the stochastic self-consistent harmonic approximation".
[Ion Errea](#), Matteo Calandra, and Francesco Mauri
- 6 **XVI International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, Trieste, Italy, 10/01/2013-12/01/2013,
"Anharmonic effects from the self-consistent harmonic approximation: the example of simple cubic calcium".
[Ion Errea](#)

- 5 **Vibrational coupling: most important, often ignored, and a challenge for ab-initio theory**, *Lausanne, Switzerland*, 06/11/2012-09/11/2012,
"Anharmonic effects from the self-consistent harmonic approximation: the example of simple cubic calcium".
Ion Errea
 - 4 **PCAM Summer School: Electronic and Optical Properties of Nanoscale Materials**, *Donostia/San Sebastián, Basque Country, Spain*, 25/06/2011-30/06/2011,
"Optical Properties of Calcium Under Pressure from First-Principle Calculations".
Ion Errea, Bruno Rousseau, Asier Eiguren, and Aitor Bergara
 - 3 **XV International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, *Trieste, Italy*, 13/01/2011-15/01/2011,
"Novel Structures, Superconductivity and Anharmonicity of Calcium Under Pressure from ab initio Calculations ".
Ion Errea and Aitor Bergara
 - 2 **Summer School on Computational Materials Sciences**,, *Donostia/San Sebastián, Basque Country, Spain*, 28/06/2010-03/07/2010,
"Superconductivity and Novel Structures of Calcium Under Pressure from ab initio Calculations".
Ion Errea and Aitor Bergara
 - 1 **46th EHPRG International Conference**, *Valencia, Spain*, 07/09/2008-12/09/2008,
"Fermi Surface Nesting and Phonon Instabilities in Simple Cubic Calcium".
Ion Errea, Miguel Martínez-Canales, Artem R. Oganov, and Aitor Bergara
- [Other Contributions to International Conferences \(presenting author underlined\)](#)
- 6 **XVII International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, *Trieste, Italy*, 15/01/2015-17/01/2015,
"First principle calculation of anharmonic effect on phonon frequency and spectral functions".
Lorenzo Paulatto, Ion Errea, Matteo Calandra, and Francesco Mauri
 - 5 **XVII International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, *Trieste, Italy*, 15/01/2015-17/01/2015,
"Ab-initio study of dynamical stability and anharmonic effects in high pressure metallic and atomic hydrogen".
Miguel Borinaga, Ion Errea, and Aitor Bergara
 - 4 **51st EHPRG International Meeting**, *London, UK*, 01/09/2013-06/09/2013,
"The emergence of low-energy plasmons under pressure induces anomalous optical properties".
Aitor Bergara, Ion Errea, Bruno Rousseau, Asier Eiguren, Idoia Garcia-Gurtubay, and Julen Ibañez-Azpiroz

- 3 **23rd AIRAPT International Conference on High Pressure Science and Technology**, *Mumbai, India*, 25/09/2011-30/09/2011,
"Anharmonic stabilization of the high pressure simple-cubic phase of calcium",
Invited.
Aitor Bergara, Ion Errea, and Bruno Rousseau
- 2 **PCAM Summer School: Electronic and Optical Properties of Nanoscale Materials**, *Donostia/San Sebastián, Basque Country, Spain*, 25/06/2011-30/06/2011,
"Magnon dispersions using TDDFT and Wannier functions".
Bruno Rousseau, Asier Eiguren, Ion Errea, and Aitor Bergara
- 1 **6th HiPSSA Meeting on the Study of Matter at Extreme Conditions (SMEC)**, *Miami, USA*, 27/03/2011-02/04/2011,
"Anharmonic stabilization of the high pressure simple-cubic phase of calcium",
Invited.
Aitor Bergara, Bruno Rousseau, and Ion Errea

Invited Seminars

- 20/05/2016 **Universidad de Oviedo**, *Oviedo, Spain*,
"Simulaciones mecánico cuánticas en hidruros superconductores a alta presión: Protones cuánticos y efectos anarmónicos".
- 03/05/2013 **Donostia International Physics Center (DIPC)**, *Donostia/San Sebastián, Basque Country, Spain*,
"Anharmonic Free Energies and Phonon Dispersions from the Self-Consistent Harmonic Approximation: The inverse isotope effect in superconducting palladium hydrides".
- 05/11/2012 **École Polytechnique fédérale de Lausanne (EPFL)**, *Lausanne, Switzerland*,
"Anharmonic effects from the self-consistent harmonic approximation: the example of simple cubic calcium".

Organization of Conferences and Workshops

- September 2018 **9th international Conference "New Generation in Strongly Correlated Electron Systems" (NGSCES2018)**, *Donostia/San Sebastián, Basque Country, Spain*, 03/09/2019-07/09/2018,
<http://ngscs2018.dipc.org/>.

Science Popularization Activities

- November 2014 **Week of Science, Technology and Innovation**, *Collaborator in the stand of Nanoscience*, Donostia/San Sebastián, Basque Country, Spain.
- Since 2014 **Collaborator in the Mapping Ignorance project**, <http://mappingignorance.org/>.
- Since 2013 **Writing a scientific blog**, <http://ionerrea.wordpress.com/blog/>.

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- November 2008, 2009, 2010 **Week of Science, Technology and Innovation**, *Collaborator in the stand of physics*, Bilbao, Basque Country, Spain.
- January 2009 **Across the Universe**, *Scientific exposition organized by AlhóndigaBilbao*, Scientific guide, Bilbao, Basque Country, Spain.
- May 2008 **Viaja a los polos**, *Scientific exposition organized by AlhóndigaBilbao*, Scientific guide, Bilbao, Basque Country, Spain.

Computer Skills

- Advanced Programming in FORTRAN90, BASH
- Intermediate Programming in PYTHON, MATHEMATICA, MATLAB
- Advanced User of QUANTUM-ESPRESSO, VASP *ab initio* codes
- Advanced User of L^AT_EX, Linux, Mac, Microsoft Windows

Languages

- Basque **Mother tongue**
- Spanish **Mother tongue**
- English **Fluent**
- French **Proficient**

written and oral fluency
oral fluency, written proficiency