

## PERSONAL INFORMATION

Dr. Elisa Jimenez-Izal

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[http://www.ehu.eus/chemistry/theory/1\\_group/elisa-jimenez/](http://www.ehu.eus/chemistry/theory/1_group/elisa-jimenez/)

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Google Scholar: WyY8GHsAAAAJ

## RESEARCH EXPERIENCE

- 2022 - now     **Associate Professor** (Prof. Adjunta)  
University of the Basque Country, UPV/EHU (Spain)
- 2019 - now     **Research Associate**  
Donostia International Physics Center, DIPC (Spain)
- 2019 - 2022    **Ikerbasque Research Fellow**  
University of the Basque Country, UPV/EHU,  
Donostia International Physics Center, DIPC (Spain)
- 2018 - 2019    **Postdoctoral Researcher.**  
University of the Basque Country, UPV/EHU (Spain)  
Advisor: Prof. Jesus M. Ugalde.
- 2016            **Postdoctoral Internship.**  
École Normale Supérieure de Lyon (France)  
Advisor: Prof. Philippe Sautet
- 2015 - 2018    **Postdoctoral Researcher.**  
University of California, Los Angeles, UCLA (USA)  
Advisor: Prof. Anastassia N. Alexandrova.
- 2010 - 2014    **PhD** in Computational Chemistry  
University of the Basque Country, UPV/EHU (Spain)  
Advisors: Jon M. Matxain and Jesus M. Ugalde.  
European doctorate, Excellent Cum laude.
- 2012            **Predoctoral Internship.**  
Departamento de Física Aplicada, CINVESTAV-IPN, Mérida (México)  
Advisor: Prof. Gabriel Merino
- 2011            **Predoctoral Internship.**  
Università degli Studi di Torino, Torino (Italy)  
Advisor: Prof. Piero Ugliengo
- 2008 - 2010    **MSc** in Computational and Theoretical Chemistry, UPV/EHU (Spain)

## FELLOWSHIPS

- 2019 - 2024 Ikerbasque Research fellowship.  
2016 - 2018 Basque Government postdoctoral fellowship.  
2010 - 2014 Basque Government predoctoral fellowship.  
2004 - 2008 Spanish Government mobility grant.

## FUNDING

### **Advanced machine-learning platform for atomistic simulations of Reactivity and Kinetics (2025-2026)**

Entity: IKUR – HPC&AI, Basque Government  
PI: Ivan Infante, Pablo Piaggi and Elisa Jimenez-Izal

### **Theoretical design of metal nanocatalysts for HOR in alkaline media (2024-2027)**

Entity: Spanish Ministry  
PI: Elisa Jimenez-Izal and Jose M. Mercero

### **Ge as key dopant to boost the catalytic performance of Pt (2021-2024)**

Entity: Spanish Ministry  
PI: Elisa Jimenez-Izal

### **Ikerbasque Research Project (2019-29/01/2024)**

Entity: Ikerbasque Science Foundation  
PI: Elisa Jimenez-Izal

## HPC PROJECTS

### 2026-2021 Computer time in Mare-Nostrum (BSC)

PI: Elisa Jimenez-Izal

### 2017 Computer time in Extreme Science and Engineering Discovery Environment (XSEDE) funded by American National Science Foundation (value of \$88.471)

PI: Anastassia Alexandrova, co-PI: Elisa Jimenez-Izal

### 2016 Computer time in Extreme Science and Engineering Discovery Environment (XSEDE) funded by American National Science Foundation (508.500 Core-hours)

PI: Anastassia Alexandrova, co-PI: Elisa Jimenez-Izal

## LIST OF PUBLICATIONS

- 1) Idoia Camara, **Elisa Jimenez-Izal**, Sara Lois, Ane Sarasola, Aran Garcia-Lekue\*  
Exploring tricoordinated graphitic oxygen as a reactivity modulator for efficient oxygen reduction catalysis  
*Submitted*
- 2) Andrea Berti, Ramón M. Bergua, Jose M. Mercero, Deborah Perco, Paolo Lacovig, Silvano Lizzit, **Elisa Jimenez-Izal**, Alessandro Baraldi\*

*Ultra-Low Atomic Diffusion Barrier on Two-Dimensional Materials: The Case of Pt on Epitaxial Graphene*

ACS Nano (2025) DOI: [10.1021/acsnano.5c13305](https://doi.org/10.1021/acsnano.5c13305)

- 3) Andoni Ugartemendia\*, Ramon M. Bergua, Jose M. Mercero, **Elisa Jimenez-Izal**  
*Boosting Synergistic Effects Between PtGe Nanoalloys and 2D Materials for PEMFC Applications*  
Int. J. Hydrog. E. **89**, 233-253 (2024). DOI: [10.1016/j.ijhydene.2024.09.279](https://doi.org/10.1016/j.ijhydene.2024.09.279)
- 4) Ramon M. Bergua, Theodoros Pavloudis, Andoni Ugartemendia, Richard E. Palmer, **Elisa Jimenez-Izal**\*  
*PdTi alloys as an excellent catalyst for semi-hydrogenation reactions*  
Appl. Surf. Sci. **672**, 160798-160805 (2024). DOI: [10.1016/j.apsusc.2024.160798](https://doi.org/10.1016/j.apsusc.2024.160798)
- 5) Xuban Gastearena, Jesus M. Ugalde, Eider San Sebastian\*, **Elisa Jimenez-Izal**\*  
*Unveiling the electronic origin of lanthanide based chiral 3D Metal Organic Framework with ideal spin filtering capacity*  
Comm. Phys. **7**, 158-163 (2024). DOI: [10.1038/s42005-024-01651-4](https://doi.org/10.1038/s42005-024-01651-4).
- 6) Silvia Escayola, **Elisa Jimenez-Izal**, Jesus M. Ugalde, Eduard Matito, Rafael Grande-Aztatzi\*, Jose M. Mercero\*  
*Unveiling the Quantum Secrets of TriaI Metal Triangles: A Tale of Stability, Aromaticity, and Relativistic Effects*  
Phys. Chem. Chem. Phys. **26**, 12619-12627 (2024). DOI: [10.1039/D4CP00484A](https://doi.org/10.1039/D4CP00484A)
- 7) Andoni Ugartemendia, Irene Casademont-Reig, Lili Zhao, Zuxian Zhang, Gernot Frenking, Jesus M. Ugalde, Aran Garcia-Lekue\*, **Elisa Jimenez-Izal**\*  
*Deciphering the chemical bond of trivalent oxygen atom in oxygen doped graphene*  
Chem. Sci. **15**, 6151-6159 (2024). DOI: [10.1039/D4SC00142G](https://doi.org/10.1039/D4SC00142G).
- 8) Andoni Ugartemendia, Jose M. Mercero, **Elisa Jimenez-Izal**, Abel de Cozar\*  
*Doping effects on ethane/ethylene dehydrogenation catalyzed by Pt<sub>2</sub>X nanoclusters*  
ChemPhysChem. **25**, e202400095-e202400105 (2024). DOI: [10.1002/cphc.202400095](https://doi.org/10.1002/cphc.202400095).
- 9) Andoni Ugartemendia, Jose M. Mercero\*, Abel de Cózar, Marco M. Melander, Jaakko Akola\*, **Elisa Jimenez-Izal**\*  
*Deposited PtGe clusters as active and durable catalysts for CO oxidation*  
ChemCatChem. **16**, e202301137-e202301150 (2024). DOI: [10.1002/cctc.202301137](https://doi.org/10.1002/cctc.202301137)
- 10) Patricia Poths, Borna Zandkarimi, Anastassia N. Alexandrova, **Elisa Jimenez-Izal**\*  
*Pt:Ge ratio as a lever of activity and selectivity control of supported PtGe clusters in thermal dehydrogenation*  
ChemCatChem **15**, e202201533-e202201543 (2023).

- 11) Andoni Ugartemendia, Aran Garcia-Lekue\*, **Elisa Jimenez-Izal\***  
*Tailoring magnetism in silicon-doped zigzag graphene edges*  
Sci. Rep. **12**, 13032-13038 (2022).
- 12) Karina G. Madrigal-Carrillo, Juan I. Rodríguez\*, Martha L. Hernández-Pichardo, **Elisa Jimenez-Izal\***  
*Unraveling the effects of Fe and Mn promoters on the tungstated zirconia catalyst: A DFT study*  
Appl. Surf. Sci. **599**, 154052-154058 (2022).
- 13) Andrea Rogolino, Nathalie Claes, Judit Cizaurre, Aimar Marauri, Alba Jumbo, Zuzanna Lawera, Joscha Kruse, María Sanromán-Iglesias, Ibai Zarketa, Unai Calvo, **Elisa Jimenez-Izal**, Yury P. Rakovich, Sara Bals, Jon M. Matxain\*, Marek Grzelczak\*.  
*Metal-polymer heterojunction in colloidal-phase plasmonic catalysis.*  
J. Phys. Chem. Lett. **13**, 2264-2272 (2022).
- 14) Andoni Ugartemendia, Jose M. Mercero\*, Abel de Cózar, **Elisa Jimenez-Izal\***. Does the Composition in PtGe Clusters Play any Role in Fighting CO Poisoning?  
J. Chem. Phys. **156**, 174301-174311 (2022).
- 15) Andoni Ugartemendia, Kristien Peeters, Piero Ferrari, Abel de Cózar, Jose M. Mercero, Ewald Janssens\*, **Elisa Jimenez-Izal\***.  
*Doping platinum with germanium: an efficient way to mitigate the CO poisoning.*  
ChemPhysChem. **22**, 1603-1610 (2021).
- 16) **Elisa Jimenez-Izal\***, Iker Ortiz de Luzuriaga, Eloy Ramos-Cordoba, Jon M. Matxain.  
*The role of dispersion interactions in endohedral TM@(ZnS)<sub>12</sub> structures.*  
ACS Omega. **6**, 16612-16622 (2021) Journal Cover. DOI: 10.1021/acsomega.1c02016
- 17) J. Vera-Iturriaga, K. G. Madrigal-Carrillo, M. L. Hernández-Pichardo, J. I. Rodríguez-Hernández, **E. Jiménez-Izal\***, J. A. Montoya de la Fuente\*.  
*A size-selective method for increasing the performance of Pt supported on tungstated zirconia catalysts for alkane isomerization: a combined experimental and theoretical DFT study*  
New J. Chem. **45**, 10510-10523. DOI: 10.1039/D1NJ01725J (2021).
- 18) Zisheng Zhang, Zhi-Hao Cui, **Elisa Jimenez-Izal**, Philippe Sautet, Anastassia N. Alexandrova\*  
*Hydrogen Evolution on Restructured B-rich WB: Metastable Surface States and Isolated Active Sites*  
ACS Catal. **10**, 13867–13877 (2020).

- 19) **Elisa Jimenez-Izal\***, Ji-Yuan Liu, Anastassia N. Alexandrova  
*Germanium as key dopant to boost the catalytic performance of small platinum clusters for alkane dehydrogenation*  
J. Catal. **374**, 93-100 (2019).
- 20) Zisheng Zhang, **Elisa Jimenez-Izal**, Ive Hermans, Anastassia N. Alexandrova\*  
*Dynamic Phase Diagram of Catalytic Surface of Hexagonal Boron Nitride in Conditions of Oxidative Dehydrogenation of Propane*  
J. Phys. Chem. Lett. **10**, 20-25 (2019).
- 21) **Elisa Jimenez-Izal**, Bruce C. Gates, Anastassia N. Alexandrova\*  
*Designing Clusters for Heterogeneous Catalysis*  
*Phys. Today* **72**, 38 (2019).
- 22) Fadel Y. Shalhout, Sergey Malyk, Joshua G. Hinman, Stephen B. Cronin, **Elisa Jimenez-Izal**, Anastassia N. Alexandrova\*, Alexander V. Benderskii\*  
*Water-Enhanced Carbon Monoxide Adsorption on Roughened Gold Surfaces in Ambient Conditions*. Submitted (2018).
- 23) Ondrej Dyck, Songkil Kim, **Elisa Jimenez-Izal**, Anastassia N. Alexandrova, Sergei V. Kalinin, Stephen Jesse\*  
*Assembling Di- and Multiatomic Si clusters in Graphene via Electron Beam*  
Small **14**, 1801771-1801779 (2018).
- 24) **Elisa Jimenez-Izal**, Huanchen Zhai, Ji-Yuan Liu, Anastassia N. Alexandrova\*  
*Nanoalloying MgO-Deposited Pt Clusters with Si for Controlling the Selectivity of Alkane Dehydrogenation*  
ACS Catal. **8**, 8346-8356 (2018).
- 25) Ivan Popov<sup>+</sup>, **Elisa Jimenez-Izal\***, Anastassia N. Alexandrova, Alexander N. Boldyrev\*  
*Multicenter Bonding Effects in Oxygen Vacancy in the Bulk and on the Surface of MgO*  
J. Phys. Chem. C **122**, 11933-11937 (2018).  
\* first-authors
- 26) J. C. Thomas, D. P. Goronzy, A. C. Serino, H. S. Auluck, O. R. Irving, **E. Jimenez-Izal**, P. Sautet, A. N. Alexandrova\*, T. Base\*, P. S. Weiss\*  
*Acid-Base Control of Valency within Carbonedithiol Self-Assembled Monolayers: Molecules Do the Can-Can*  
ACS Nano **12**, 2211-2221 (2018).

- 27) **Elisa Jimenez-Izal**, Anastassia N. Alexandrova\*  
*Computational Design of Clusters for Catalysis*  
Annual Rev. Phys. Chem. **69**, 377-400 (2018). Invited article
- 28) Zhihao Cui, **Elisa Jimenez-Izal**, Anastassia N. Alexandrova\*  
*Prediction of Two-dimensional Phase of Boron with Anisotropic Electric Conductivity*  
J. Phys. Chem. Lett. **8**, 1224-1228 (2017).
- 29) **Elisa Jimenez-Izal**, Mark Saeys, Anastassia N. Alexandrova\*  
*Metallic and Magnetic 2D Materials Containing Planar Tetracoordinated C and N*  
J. Phys. Chem. C, Mark Gordon's Festschrift issue, **120**, 21685-21690 (2016).
- 30) **Elisa Jimenez-Izal**, Anastassia N. Alexandrova\*  
 *$\sigma$ -Aromaticity in Polyhydride Complexes of Ru, Ir, Os, and Pt*  
Phys. Chem. Chem. Phys. **18**, 11644-11652 (2015). Invited article for the special issue on aromaticity.
- 31) Jonny Dadras, **Elisa Jimenez-Izal**, Anastassia N. Alexandrova\*  
*Alloying Pt Sub-Nano-Clusters with Boron: Sintering Preventative and Coke Antagonist?*  
ACS Catal. **5**, 5719-5727 (2015).
- 32) **Elisa Jimenez-Izal**, Jesus M. Ugalde, Jon M. Matxain\*  
*Nanocluster-assembled Materials* Chapter from the Book *Computational Modeling of Inorganic Nanomaterials*  
4. chapter 113-148. Editors: Stefan T. Bromley and Martjin A. Zwinenburgh  
Publisher: CRC Press, Taylor & Francis Group. Series in Materials Science and Engineering (2016). LCCN 2016003208; ISBN 9781466576414 (alk. Paper), ISBN 1466576413 (alk. Paper).
- 33) **Elisa Jimenez-Izal\***, Jose M. Mercero, Jon M. Matxain, Martha Audiffred, Diego Moreno, Gabriel Merino\*, Jesus M. Ugalde  
*Doped Aluminum Cluster Anions: Size Matters*  
J. Phys. Chem. A **118**, 4309-4314 (2014).
- 34) **Elisa Jimenez-Izal\***, Jon M. Azpiroz, Riti Gupta, Jon M. Matxain, Jesus M. Ugalde  
*CdS Nanoclusters Doped with Divalent Atoms*  
J. Mol. Model. **20**, 2227-2239 (2014).
- 35) **Elisa Jimenez-Izal\***, Jon M. Matxain, Mario Piris, Jesus M. Ugalde  
*Second-row transition-Metal Doping of  $(Zn_iS_i)_{i=12,16}$  Nanoclusters. Structural and Magnetic Properties*  
Computation **1**, 31-45 (2013).

- 36) Stefan M. Huber\*, Joseph D. Scanlon, **Elisa Jimenez-Izal**, Jesus M. Ugalde, Ivan Infante\*  
*On the Directionality of Halogen Bonding*  
Phys. Chem. Chem. Phys. **15**, 10350-10357 (2013).
- 37) **Elisa Jimenez-Izal**, Fabio Chiatti, Marta Corno, Albert Rimola, Piero Ugliengo\*  
*Glycine Adsorption at Nonstoichiometric (010) Hydroxyapatite Surfaces: A B3LYP Study*  
J. Phys. Chem. C **116**, 14561-14567 (2012).
- 38) Stefan M. Huber\*, **Elisa Jimenez-Izal**, Jesus M. Ugalde, Ivan Infante\*  
*Unexpected Trends in Halogen-Bond Based Noncovalent Adducts*  
Chem. Comm. **48**, 7708-7710 (2012).
- 39) **Elisa Jimenez-Izal**\*, Jon M. Matxain, Mario Piris, and Jesus M. Ugalde  
*Self-assembling endohedrally doped CdS nanoclusters: new porous solid phases of CdS*  
Phys. Chem. Chem. Phys. **14**, 9676-9682 (2012).
- 40) **Elisa Jimenez-Izal**\*, Jon M. Matxain, Mario Piris, and Jesus M. Ugalde  
*Thermal Stability of Endohedral First-Row Transition-Metal  $TM@Zn_iS_i$  Structures,  $i=12,16$*   
J. Phys. Chem. C **115**, 7829-7835 (2011).
- 41) **Elisa Jimenez-Izal**\*, Jon M. Matxain, Mario Piris, Jesus M. Ugalde  
*Structure and Stability of the Endohedrally Doped ( $X@CdS$ )  $X=Na,K,Cl,Br$  Nanoclusters*  
J. Phys. Chem. C **114**, 2476-2483 (2010).

## INVITED LECTURES

- 2022 DIPC Community Seminar  
[\*Size and composition effects in heterogeneous catalysis through the electronic structure insight\*](#)
- 2018 Instituto Politécnico Nacional - Ciudad de México  
*Tuning the electronic properties of Pt catalysts*
- 2018 Donostia International Physics Center  
*Computational materials chemistry: heterogeneous nanocatalysts and 2D materials*
- 2017 University of Southern California - Los Angeles  
*Computational design of functional materials*

## PARTICIPATION IN CONFERENCES

- 1) Clusters Surface Interaction 2026, Paris, France (2026). **Invited lecture** *Transition-metal nanoalloys in hydrogenation and dehydrogenation reactions.*
- 2) Basque Catalysis Symposium, Donostia, Spain (2026). **Invited lecture** *Tailoring graphene for advanced catalytic applications.*
- 3) Electronic Structure: Prediction and Applications 2024, Tarragona, Spain (2024). **Oral presentation** *An exotic way for oxygen to dope graphene.*
- 4) Cluster Meeting 2023 Prague, Czech Republic (2023). **Hot Topic talk** *Pt:Ge ratio as a lever of activity and selectivity control of PtGe clusters.*
- 5) ZCAM and CECAM: Present & Future, Zaragoza (2023). **Poster** *Tailoring PtGe catalysts for target reactions.*
- 6) Workshop "From bioinorganic chemistry to catalysis" Donostia, Basque Country (2023). **Invited lecture** *Looking for the most durable heterogeneous catalysts by playing with the composition.*
- 7) International Conference on Chemical Bonding, Kauai, USA (2022). **Invited lecture** *Understanding novel catalysts through chemical bonding analysis.*
- 8) International Conference on Theoretical Aspects of Catalysis (ICTAC), Lyon, France (2022). **Oral presentation** *Making Pt highly CO-tolerant and highly active for hydrogen oxidation.*
- 9) 2<sup>nd</sup> Global Virtual Summit on Catalysis & Chemical Engineering, Virtual (2022). **Invited lecture (keynote speaker)** *Theoretical Design of CO-tolerant Catalysts for Fuel Cells.*
- 10) Symposium of the Spanish Royal Society of Chemistry, Virtual (2021). **Oral presentation** *Doping Pt with Ge: a novel way to mitigate the CO poisoning.*
- 11) International Meeting on Nanoalloys (IMN 2021), Virtual (2021). **Oral presentation** *Nanoalloying Pt with Ge to obtain highly selective catalysts.*
- 12) 8th Edition of Global Conferences on Catalysis, Global Engineering & Technology, Virtual (2020). **Invited lecture** *Boosting the selectivity of Pt through Ge doping.*
- 13) XXXVII Bienal de la Real Sociedad Española de Química (RSEQ), Donostia, Spain (2019). **Oral presentation** *Computational Design of Pt-based nanocatalysts.*
- 14) Theoretical Chemistry and Computational Modeling: 20 years promoting Excellence in Science, Donostia, Spain (2019). **Poster** *Novel 2D materials: Computational prediction.*
- 15) Transborder QuantumChemPhys Lab Meeting, Baiona, France (2108). **Invited lecture** *Nanoalloying MgO-deposited Pt clusters with Si for controlling the selectivity of alkane dehydrogenation.*
- 16) Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy, Donostia, Spain (2018). **Poster** *Theoretical predictions of novel 2D materials with unique electronic properties.*
- 17) 16th International Congress of Quantum Chemistry, Menton, France (2018). **Poster** *Improving the durability of Pt nanocatalysts for alkane dehydrogenation.*

- 18) Main Group Chemistry Symposium, Los Angeles, USA (2017). **Oral presentation** *Main group elements in 2D materials*.
- 19) XV Reunión Mexicana de Fisicoquímica Teórica, Mérida, México (2016). **Invited lecture** *Estabilización de nanoclusters de Pt como catalizadores*.
- 20) Seaborg Symposium, California NanoSystems Institute (CNSI), Los Angeles, USA (2016). **Poster** *Prediction of new 2D materials with exotic electronic properties*.
- 21) Electronic Structure: Prediction and Applications 2016, Castellón, Spain (2016). **Invited lecture** *Metallic nanoclusters as catalysts: towards a greener chemistry*.
- 22) Cluster Surface Interaction Workshop 2016 Argonne National Lab, Chicago (2016). **Hot topic talk** *Can we Design Highly Stable Metallic Nanoclusters for their Use in Heterogeneous Catalysis?*
- 23) ACS National Meeting, San Diego, USA (2016). **Poster** *Improvement of platinum nanocatalysts via boron doping*.
- 24) ACS National Meeting, San Diego, USA (2016). **Oral presentation** *Sub-nano surface-deposited Pt cluster catalysts: realistic modeling and tuning through the electronic structure insight*.
- 25) Seaborg Symposium, California NanoSystems Institute (CNSI), Los Angeles, USA (2015). **Poster** *Stabilization of Pt nanoclusters for their use as heterogeneous catalysts*.
- 26) XI Reunión Mexicana de Fisicoquímica Teórica, Toluca de Lerdo, México (2012). **Oral presentation** *Diseño de sólidos nanoporosos basados en nanoclusters CdS dopados endohédricamente*.
- 27) Modelling Realistic Inorganic Nanostructures: bridging the gap between theory and experiment, Zaragoza, Spain (2012). **Invited lecture** *Designed porous solids based on endohedrally doped CdS nanoclusters*.
- 28) Jornada Universitaria de Matemáticas en Otras Ciencias, Bilbao, Spain (2012). **Oral presentation** *Las matemáticas de la química teórica y computacional*.
- 29) Electronic Structure: Prediction and Applications 2012, Barcelona, Spain (2012). **Poster** *Designed porous solids based on endohedrally doped CdS nanoclusters*.
- 30) Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms, Sigüenza, Spain (2011). **Poster** *Bond energy decomposition of the interaction between Iodoperfluoroarenes and halide anions*.
- 31) The World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain (2011). **Poster** *Designing porous solids based on endohedrally doped CdS nanoclusters*.
- 32) Electronic Structure: Prediction and Applications 2010, Oviedo, Spain (2010). **Poster** *Thermal stability of endohedrally doped first-row transition-metal TM@Zn<sub>n</sub>S<sub>i</sub> structures, i=12, 16*.
- 33) Electronic Structure: Prediction and Applications 2008, Mallorca, Spain (2008). **Poster** *Endohedral (X@Cd<sub>n</sub>S<sub>n</sub>)<sup>q</sup> nanoclusters, X= Li, Na, K, F, Cl, Br; n= 4, 9, 12, 15, 16; q= -1, 0, 1*.

## SUPERVISION OF STUDENTS

### Ongoing

- Ramon Bergua. **PhD thesis**  
*Theoretical study of electronic, structural and environmental effects in precious-metal nanocatalysts*  
Supervisors: Elisa Jimenez-Izal and Jose M. Mercero, UPV/EHU.
- Idoia Camara. **PhD thesis**  
Supervisors: Jose M. Mercero and Elisa Jimenez-Izal, UPV/EHU.
- Aritz Echevarria. Final thesis Bachelor degree  
Supervisors: J. M. Mercero, Elisa Jimenez-Izal UPV/EHU.

### Past

- Idoia Camara. **Master thesis**  
*Evaluating PtGe surface as a Catalyst for Hydrogen Evolution: calculations of Voltage-Dependent Activation Energy*  
Supervisors: Jose M. Mercero and Elisa Jimenez-Izal, UPV/EHU (25/09/2025).
- Andoni Ugartemendia. **PhD thesis**  
*Computational design of CO-poisoning resistant Pt catalysts.*  
Supervisors: Elisa Jimenez-Izal and Jose M. Mercero, UPV/EHU (01/03/2024).
- Unai Polo. Final thesis Bachelor degree  
*Evaluación del carácter multi configuracional en catalizadores de Pt para la reacción de deshidrogenación de etano*  
Supervisors: J. M. Mercero, Elisa Jimenez-Izal UPV/EHU (2024).
- Idoia Camara. Final thesis Bachelor degree  
 *$B_nX_m$  ( $n= 7-10$ ,  $m= 1-3$ ,  $X= Au, Li, Bi$ ) molekulen gainazal potentzialaren azterketa, nanozinten bila*  
Supervisors: Jose M. Mercero and Elisa Jimenez-Izal, UPV/EHU (September 2023).
- Karina G. Madrigal. **PhD thesis**  
*Zirconia supported  $WO_3$  catalysts for n-hexane isomerization: theoretical study.*  
Escuela Superior de Física y Matemáticas, Instituto Politécnico Nacional (México).  
Supervisors: Elisa Jimenez-Izal and Juan I. Rodriguez (15/11/2022)
- Sara Navarro. Final thesis Bachelor degree  
*Theoretical study of oxygen doped graphene with potential applications in electronic devices.*  
Supervisors: J. Feuchtwanger, E. Jimenez-Izal, A. Garcia-Lekue, UPV/EHU (2022).
- Xuban Gastearena. **Master thesis**  
*Computational characterization of electronic properties of chiral Metal Organic Frameworks. Understanding the spin dependent electron conductivity and the Chiral Induced Spin Selectivity (CISS) Effect.*  
Supervisors: Eider San Sebastian and Elisa Jimenez-Izal, UPV/EHU (2022).

- Asier Murillo. Final thesis Bachelor degree  
*Design of atomic scale graphene-based materials for their use in electronic devices*  
Supervisors: J. M. Mercero, Elisa Jimenez-Izal, Aran Garcia-Lekue, UPV/EHU (2021).
- Andoni Ugartemendia. **Master thesis**  
*Computational design of CO-poisoning resistant Pt catalysts*  
Supervisors: Elisa Jimenez-Izal and Jose M. Mercero, UPV/EHU (24/07/2020).
- Ibai Zarketa. Final thesis Bachelor degree  
*Structure and semiconducting properties of PTEBS polymer*  
Jon M. Matxain and Elisa Jimenez-Izal, UPV/EHU (2019).
- Andoni Ugartemendia. Final thesis Bachelor degree  
*Doping Pt catalysts to reduce their deactivation*  
Supervisors: Jon M. Matxain and Elisa Jimenez-Izal, UPV/EHU (2018).

## TEACHING

<u>2020 - present</u>	Kimika Fisikoa II
<u>2023 - 2024</u>	Experimental Physical Chemistry
<u>2018 - 2019</u>	Metodologia Experimentala Kimikan

## OUTREACH ACTIVITIES

- Ciclo Cine y Ciencia, Madame Curie **Presentation** Donostia & Iruña (2023).
- 10th Meeting of Scientific Lives with High School Students, Eureka Museum of Science  
**Poster presentation** (2021).
- 10th Meeting of Scientific Lives with High School Students, Eureka Museum of Science  
**Invited talk** (2021).
- Women Scientist of Yesterday and Today* organized by the local government of San Sebastian **Invited talk** (2021).  
[▶ WeekINN TV | Mujeres científicas de ayer y hoy](#)
- Women Scientist of Yesterday and Today* organized by *Women in Science* **Invited talk** (2021).  
[▶ 2021 - Emakume Zientzialariak Atzo eta Gaur | Científicas de ayer y de hoy](#)
- School of applied ethics: Ethics and good professional practices in contemporary society* conference organized by UPV/EHU (2014).
- First meeting to promote scientific culture* conference organized by UPV/EHU (2014).
- The social impact of science and the role of the media* conference organized by UPV/EHU (2010).

## INSTITUTIONAL RESPONSIBILITIES

- Since September 2025: Member of CURES (RES Users Committee)
- Since 20/12/2023: Miembro Comisión Académica del Master *Theoretical Chemistry and Computational Modelling*
- February 2019 - June 2025: Member of the Equality Committee of the Donostia International Physics Center (DIPC)
- May 2021 - February 2023: Member of the Equality Commission at the Chemistry Department of UPV/EHU

## PARTICIPATION IN WORKSHOPS

- Ab initio Modeling in Solid State Chemistry*, Torino, Italy (2011).
- Photoeffects at Semiconductors for Energy and Environment*, Torino, Italy (2011).
- Quantum Monte Carlo and the CASINO program V*, Tuscany, Italy (2010).
- A hands on tutorial on the SIESTA code*, Santander, Spain (2010).
- Spring College on Computational Nanoscience*, Trieste, Italy (2010).
- Electronic structure calculations in solid state*, Oviedo, Spain (2009).

## OTHERS

**Certificado I3** concedido por la Secretaría General de Universidades  
Programa de Incentivación de la Incorporación e Intensificación de la Actividad Investigadora  
(Programa I3)

## MEMBER OF SCIENTIFIC BOARD

Cluster-Surface Interactions

## ORGANIZING COMMITTEE

XIX International Conference on Theoretical Aspects of Catalysis (ICTAC) 2024

## SCIENTIFIC SERVICES AS REVIEWER

ACS Catal. (ACS), Phys. Chem. Chem. Phys. (RSC), Nanoscale (RSC), Chem. Phys. Lett. (Elsevier), J. Mol. Model. (Springer), Theoretical Chemistry Accounts (Springer), J. Theor. Comput. Chem. (World Scientific), Computation (MDPI), AIChE J. (Wiley), J. Phys. Chem (ACS), Catal. Sci. Technol (RSC), Appl. Surf. Sci. (Elsevier), Appl. Cat. B - Env. (Elsevier).

## LANGUAGE SKILLS

Spanish and Basque: mother tongue (bilingual); English: fluent.