PERSONAL INFORMATION

Dr. Elisa Jimenez-Izal
Email: elisa.jimenez@ehu.es
ORCID: 0000-0003-1127-2100
Google Scholar: WyY8GHsAAAAJ
http://www.ehu.eus/chemistry/theory/1_group/elisa-jimenez/
https://www.ikerbasque.net/es/elisa-jimenez-izal

RESEARCH EXPERIENCE

2019 - now **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)
Structure and Electronic Properties of Endohedrally Doped II-VI Hollow Nanoclusters
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

Ge as key dopant to boost the catalytic performance of Pt (2021-2023)
Entity: Spanish Ministry
Ikerbasque Research Project
Entity: Ikerbasque Science Foundation

HPC PROJECTS

2022 Computer time in Mare-Nostrum (BSC) (2.764 Kh)
PI: Elisa Jimenez-Izal

2021 Computer time in Mare-Nostrum (BSC) (2.764 Kh)
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

2016 Computer time at the EMSL of the Pacific Northwest National Lab. funded by the American Department of Energy (100.000 Core-hours).
PI: Anastassia Alexandrova

2015 Computer time at the EMSL of the Pacific Northwest National Lab. funded by the American Department of Energy (100.000 Core-hours).
PI: Anastassia Alexandrova

LIST OF PUBLICATIONS

1) 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).

2) Andoni Ugartemendia, Jose M. Mercero, Abel de Cózar, **Elisa Jimenez-Izal***. Does the *Composition in PtGe Clusters Play any Role in Fighting CO Poisoning?*
Submitted

3) 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).

4) **Elisa Jimenez-Izal***, Iker Ortiz de Luzuriaga, Eloy Ramos-Cordoba, Jon M. Matxain.
The role of dispersion interactions in endohedral TM@$(ZnS)_{12}$ structures.
ACS Omega. **6**, 16612-16622 (2021) Journal Cover. DOI: 10.1021/acsomega.1c02016

5) 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).

6) 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).

7) **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).

8) 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).

9) **Elisa Jimenez-Izal**, Bruce C. Gates, Anastassia N. Alexandrova*
Designing Clusters for Heterogeneous Catalysis
Phys. Today **72**, 38 (2019).

10) 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).

11) 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).

12) **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).

13) Ivan Popov[+], **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

14) 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).

15) **Elisa Jimenez-Izal**, Anastassia N. Alexandrova*
Computational Design of Clusters for Catalysis
Annual Rev. Phys. Chem. **69**, 377-400 (2018). Invited article

16) 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).

17) **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 Festchrift issue*, **120**, 21685-21690 (2016).

18) **Elisa Jimenez-Izal**, Anastassia N. Alexandrova*
σ-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.

19) 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).

20) **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. Zwinenburg
Publisher: CRC Press, Taylor & Francis Group. Series in Materials Science and Engineering (2016). LCCN 2016003208; ISBN 9781466576414 (alk. Paper), ISBN 1466576413 (alk. Paper).

21) **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).

22) **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).

23) **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).

24) 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).

25) **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).

26) 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).

27) **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).

28) **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).

29) **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) International Conference on Chemical Bonding, Kauai, USA (2022). **Invited lecture**
2) International Conference on Theoretical Aspects of Catalysis (ICTAC), Lyon, France (2022). **Oral presentation** *Making Pt highly CO-tolerant and highly active for hydrogen oxidation.*
3) 2nd Global Virtual Summit on Catalysis & Chemical Engineering, Virtual (2022). **Invited lecture (*keynote speaker*)** *Theoretical Design of CO-tolerant Catalysts for Fuel Cells.*
4) Symposium of the Spanish Royal Society of Chemistry, Virtual (2021). **Oral presentation** *Doping Pt with Ge: a novel way to mitigate the CO poisoning.*

5) International Meeting on Nanoalloys (IMN 2021), Virtual (2021). **Oral presentation** *Nanoalloying Pt with Ge to obtain highly selective catalysts.*
6) 8th Edition of Global Conferences on Catalysis, Global Engineering & Technology, Virtual (2020). **Invited lecture** *Boosting the selectivity of Pt through Ge doping.*
7) XXXVII Bienal de la Real Sociedad Española de Química (RSEQ), Donostia, Spain (2019). **Oral presentation** *Computational Design of Pt-based nanocatalysts*.
8) Theoretical Chemistry and Computational Modeling: 20 years promoting Excellence in Science, Donostia, Spain (2019). **Poster** *Novel 2D materials: Computational prediction*.
9) Transborder QuantumChemPhys Lab Meeting, Baiona, France (2108). **Invited lecture** *Nanoalloying MgO-deposited Pt clusters with Si for controlling the selectivity of alkane dehydrogenation.*
10) Novel 2D Materials Explored via Scanning Probe Microscopy & Spectroscopy, Donostia, Spain (2018). **Poster** *Theoretical predictions of novel 2D materials with unique electronic properties.*
11) 16th International Congress of Quantum Chemistry, Menton, France (2018). **Poster** *Improving the durability of Pt nanocatalysts for alkane dehydrogenation.*
12) Main Group Chemistry Symposium, Los Angeles, USA (2017). **Oral presentation** *Main group elements in 2D materials*.
13) XV Reunión Mexicana de Fisicoquímica Teórica, Mérida, México (2016). **Invited lecture** *Estabilización de nanoclusters de Pt como catalizadores*.
14) Seaborg Symposium, California NanoSystems Institute (CNSI), Los Angeles, USA (2016). **Poster** *Prediction of new 2D materials with exotic electronic properties*.
15) Electronic Structure: Prediction and Applications 2016, Castellón, Spain (2016). **Invited lecture** *Metallic nanoclusters as catalysts: towards a greener chemistry*.
16) 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?*
17) ACS National Meeting, San Diego, USA (2016). **Poster** *Improvement of platinum nanocatalysts via boron doping*.
18) 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*.
19) Seaborg Symposium, California NanoSystems Institute (CNSI), Los Angeles, USA (2015). **Poster** *Stabilization of Pt nanoclusters for their use as heterogeneous catalysts*.
20) XI Reunión Mexicana de Fisicoquímica Teórica, Toluca de Lerdo, México (2012). **Oral presentation** *Diseño de sólidos nanoporosos basados en nanoclusters CdS dopados endohédricamente*.
21) 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*.
22) Jornada Universitaria de Matemáticas en Otras Ciencias, Bilbao, Spain (2012). **Oral presentation** *Las matemáticas de la química teórica y computacional*.

23) Electronic Structure: Prediction and Applications 2012, Barcelona, Spain (2012). **Poster** *Designed porous solids based on endohedrally doped CdS nanoclusters*.
24) 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*.
25) The World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain (2011). **Poster** *Designing porous solids based on endohedrally doped CdS nanoclusters*.
26) Electronic Structure: Prediction and Applications 2010, Oviedo, Spain (2010). **Poster** *Thermal stability of endohedrally doped first-row transition-metal TM@Zn_iS_i structures, i=12, 16*.
27) Electronic Structure: Prediction and Applications 2008, Mallorca, Spain (2008). **Poster** *Endohedral (X@Cd_nS_n)^q nanoclusters, X= Li, Na, K, F, Cl, Br; n= 4, 9, 12, 15, 16; q= -1, 0, 1*.

SUPERVISION OF STUDENTS

Ongoing

- ☐ 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: Juan I. Rodriguez and Elisa Jimenez-Izal.
- ☐ Andoni Ugartemendia. **PhD thesis**
  Computational design of CO-poisoning resistant Pt catalysts.
  Supervisors: Elisa Jimenez-Izal and Jose M. Mercero, UPV/EHU.
- ☐ Xuban Gastearena. **Master thesis**
  Computational analysis of the electronic, optical and catalytic properties of two and three-dimensional MOFs with application in the energy sector. UPV/EHU
  Supervisors: Eider San Sebastian and Elisa Jimenez-Izal, UPV/EHU
- ☐ Sara Navarro. Final thesis Bachelor degree
  Supervisors:Jorge Feuchtwanger, Aran Garcia-Lekue, Elisa Jimenez-Izal, UPV/EHU

Past

- ☐ 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 (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

2020 - present Praktikak Kimika Fisikoan II (2.5 kredito) 2020-2021 ikasturtea
2018 - 2019 Metodologia Experimentala Kimikan (2 kredito)

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).

OUTREACH ACTIVITIES

- ☐ 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 Emakume* **Invited talk** (2021).
  2021 - Emakume Zientzialariak Atzo eta Gaur | Científicas de ayer y de hoy
- ☐ Member of the Equality Committee of the Donostia International Physics Center (DIPC)
- ☐ member of the Equality Commission at the Chemistry Department of UPV/EHU
- ☐ *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).

PARTICIPATION IN WORKSHOPS

- ☐ “How to Write a H2020 Proposal for MCSA Individual Fellowships”, Gasteiz (2014).
- ☐ "Ab initio Modelling 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).
- ☐ “Basic introduction to the use of Arina”, Donostia, Spain (2008).

LANGUAGE SKILLS

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