



Elena Formoso Estensoro

Curriculum Vitae

Personal Information

Last Name/ First Name Formoso, Elena
Nationality Spanish
Date of birth January 14th, 1981

Education

- 2010 **PhD. in Computational and Theoretical Chemistry (Doctor Europeus)**, *University of the Basque Country (UPV/EHU)*, Donostia, Spain.
Dissertation: Theoretical Characterization of Pentacovalent Oxyphosphorane Intermediate Structures of the Hydrolysis of RNA Catalyzed by RNase A.
Grade: Sobresaliente Cum Laude. Supervisor: Prof. X. Lopez
Examining Committee:
○ Prof. Darrin M. York, *University of Minnesota*, Minneapolis, USA
○ Prof. Annick Dejaegere, *University of Strasbourg*, Strasbourg, France
○ Prof. Rita Guedes, *University of Lisbon*, Lisbon, Portugal
○ PhD. Elixabete Rezabal, *Johann Wolfgang Goethe, University of Frankfurt*, Frankfurt am Main, Germany
○ PhD. Eider San Sebastian, *Ikerchem Ltd.*, Donostia, Euskadi, Spain
- 2006 **Diploma of Advanced Studies in Computational Chemistry**, *University of the Basque Country (UPV/EHU)*, Donostia, Spain.
- 2004 **Licenciature in Chemistry**, *University Autonoma of Madrid (UAM)*, Madrid, Spain.
Extraordinary award

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Work Experience

Contracts and Fellowships

- Feb 2014 – present **Postdoctoral Research Associate**, *Donostia International Physics Center (DIPC)*, Donostia, Spain.
Group of Prof. Jesus M. Ugalde
- Feb 2011 – Jan 2014 **ETH Postdoctoral Research Associate**, *Department of Chemistry and Applied Biosciences, Institute of Computational Sciences, Università della Svizzera Italiana (USI) and ETH Zurich*, Lugano, Switzerland.
Group of Prof. Michele Parrinello
- 2011–2013 **Postdoctoral Research Fellowship from the Government of the Basque Country**, *Institute for Computational Molecular Science, Temple University*, Philadelphia, USA.
Group of Prof. Michael L. Klein.
Renounce
- Sep 2009 – Jan 2011 **Graduate Research**, *Theoretical Chemistry Group, Department of Chemistry, University of the Basque Country (UPV/EHU)*, Donostia, Spain.
Group of Prof. Jesus M. Ugalde
- Sep 2005 – Aug 2009 **Pre-doctoral Fellowship from the Spanish Education and Science Office**, *Theoretical Chemistry Group, Department of Chemistry, University of the Basque Country (UPV/EHU)*, Donostia, Spain.
Group of Prof. Jesus M. Ugalde
- 2005 **Fellowship for Doctoral Studies from the Spanish Education and Science Office**, Spain.
- Sep 2003 – Jun 2004 **Undergraduate Research Fellowship from the Government of the Basque Country**, *Department of Chemistry, University Autonoma of Madrid (UAM)*, Madrid, Spain.
Group of Prof. Manuel Yañez

Stays in Foreign Centers

- Mar 2008–May 2008 **Visiting Graduate Researcher**, *School of Chemistry, University of Bristol*, Bristol, England.
Supervisor: Prof. Adrian Mulholland.
Duration: 3 month
- Mar 2007–May 2007 **Visiting Graduate Researcher**, *Department of Chemistry, University of Minnesota*, Minneapolis, USA.
Supervisor: Prof. Darrin M. York.
Duration: 3 month

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Jun 2006 – Sep 2006 **Visiting Graduate Researcher**, Department of Chemistry, University of Minnesota, Minneapolis, USA.
Supervisor: Prof. Darrin M. York.
Duration: 3 month

Scientific Meetings, Congresses and Proceedings

Invited Oral Presentations

- March 1, 2015 **11th Keele Meeting on Aluminum. The Natural History of Aluminum: Past, Present and Future**, *Effect of Al(III) on coenzyme NADH in solution*, Lille, France.
- June 20, 2014 **1st BCAM Workshop on Nonlinear dynamics in Biological Systems**, *Pulling back the curtain on the Adenylate Kinase functional mechanism*, Bilbao, Spain.
- June 25, 2013 **6th International Theoretical Biophysics Symposium (TheoBio 2013)**, *The Energy Landscape of Adenylate Kinase Modulated by Mg, ATP and AMP*, Gothenburg, Sweden.
- September 20, 2010 **Faculty of Informatics, Università della Svizzera italiana (USI)**, *Theoretical Characterization of Pentacovalent Oxyphosphorane Intermediate Structures of the Hydrolysis of RNA Catalyzed by RNase A*, Lugano, Switzerland.
- July 1, 2009 **4th International Theoretical Biophysics Symposium (TheoBio 2009)**, *Thio effects on molecular dynamics simulation of RNase A - CpA Transition State like complexes*, Roscoff, France.
- March 23, 2009 **Faculty of Science and Technology, University of the Basque Country (UPV/EHU)**, *La Ciencia desde la Perspectiva de la Universidad, la Sociedad y la Empresa*, Bilbao, Spain.
- December 18, 2008 **19 Conferencia de Química**, *Rotura Hidrolítica de Enlaces Fosfodiéster en la RNasa A*, Santiago de Cuba, Cuba.
- June 18, 2007 **3rd Symposium on Theoretical Biophysics (TheoBio 2007)**, *Hydrolytic Cleavage of Phosphodiester Bonds*, Cetraro, Italy.

Posters

- June 8, 2015 **7th International Theoretical Biophysics Symposium (TheoBio 2015)**, *Effect of Al(III) on coenzyme NADH in solution*, Cagliari, Italy.
- March 12, 2014 **Long Time Dynamics from Short Time Simulations, CECAM Workshop**, *Insight into the Adenylate Kinase functional mechanism: energetics characterization and mapping the druggable spots*, Lugano, Switzerland.

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- July 22, 2011 **9th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011)**, *Thio effects on the solvation and enzyme-ligand interactions of RNase A-CpA Complex*, Santiago de Compostela, Spain.
- October, 2010 **8th RNase Congress**, *Thio effects on Molecular Dynamics Simulation of RNase A – CpA Transition State-like Complexes*, Naples, Italy.
- July 19, 2010 **7th Congress on Electronic Structure: Principles and Applications (ESPA 2010)**, *Thio effects on Molecular Dynamics Simulation of RNase A – CpA Transition State-like Complexes*, Oviedo, Spain.
- September, 2008 **6th Congress on Electronic Structure: Principles and Applications (ESPA 2008)**, *Hydrolytic Cleavage of Phosphodiester Bonds in RNase A Ribonuclease*, Palma de Mallorca, Spain.
- May, 2006 **Conference on Isolated Biomolecules and Biomolecular Interactions (IBBI 2006)**, *Stochastic Boundary Molecular Dynamics Simulation of GDP + Pi + RAB-11 Complex*, Trest, Czech Republic.
- March, 2006 **3rd NanoSpain Workshop**, *Endohedral $(X@Zn_nS_n)^q$ Clusters, $X=Li,Na,K,F,Cl,Br$, $n=4-16$, $q=0,1,-1$* , Pamplona, Spain.
- June, 2005 **2nd Theoretical Biophysics Symposium (TheoBio 2005)**, *Stochastic Boundary Molecular Dynamics Simulation of GDP + Pi + RAB-11 Complex*, Örebro, Sweden.

Assistance

- June, 2013 **7th Molecular Quantum Mechanics (MQM)**, Lugano, Switzerland.
- January, 2011 **Pacific Symposium on Biocomputing 2011**, Big Island of Hawaii, USA.
- September, 2004 **Electronica Structure: Principles and Applications (ESPA2004)**, Valladolid, Spain.

Participation in Funded Projects

As Principal Investigator

- 2013 – 2014 **Simulation of Large Scale Conformational Fluctuations in Adenylate Kinase**, Principal Investigator: Elena Formoso, Swiss National Supercomputing Centre (CSCS), S358, 45000 chf.
Project design and development

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2012 – 2013 **Simulation of Large Scale Conformational Fluctuations in Adenylate Kinase**, *Principal Investigator: Elena Formoso*, Swiss National Supercomputing Centre (CSCS), S358, 44100 chf.
Project design and development

As member of the Investigator Team

2016 – 2019 **Estudio Computacional del Aluminio en Sistemas Biológicos: Caracterización de Compuestos y Mecanismo Molecular de su Toxicidad**, *Principal Investigator: Prof. X. Lopez, M. Piris*, Spanish Ministry of Economy and Competitiveness (MINECO), CTQ2015-67608-P, 83300 €.
Project development

2014 – 2018 **Efectos del Aluminio en Sistemas Biológicos: Una Aproximación Computacional**, *Principal Investigator: Prof. X. Lopez*, University of the Basque Country (UPV/EHU), PES14/35, 34586.39 €.
Project development

2013 – 2018 **Avances Química Cuántica**, *Principal Investigator: Prof. J. Ugalde*, Government of the Basque Country, IT588-13, 401598 €.
Project development

2013 – 2015 **Interacción del Aluminio(III) con Bioligandos y Efectos Radicales en Biomoléculas**, *Principal Investigator: Prof. X. Lopez*, Spanish Ministry of Economy and Competitiveness (MINECO), CTQ2012-38496-C05-04, 28000 €.
Project development

2011 – 2014 **Aptamers: a new frontier in drug design**, *Principal Investigator: Prof. Michele Parrinello*, Private Foundation, 784800 chf.
Project development

2010 – 2011 **Nanopartículas semiconductoras en entorno biológico: aplicaciones biomédicas?**, *Principal Investigator: Prof. X. Lopez*, Government of the Basque Country, SAIOTEK program, S-PC10UN04, 54188.03 €.
Project development

2009 – 2011 **Avances en Química Cuántica y su Aplicación a Problemas Seleccionados de Nanotecnología y Bioquímica**, *Principal Investigator: Prof. J. Ugalde*, Spanish Science and Technology Office (MCYT), CTQ2008-05739, 181999.99 €.
Project development

2007 – 2012 **Avances en Química Cuántica**, *Principal Investigator: Prof. J. Ugalde*, Government of the Basque Country, IT330-07, 438176.61 €.
Project development

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- 2007 – 2008 **Ensamblado de nanoclusters: desarrollo de nuevos materiales semiconductores y magnéticos nanoporosos**, *Principal Investigator: Prof. J. Ugalde*, Government of the Basque Country, SAIOTEK program, 45000.00 €.
Project development
- 2006 – 2007 **Ensamblado de nanoclusters: desarrollo de nuevos materiales semiconductores**, *Principal Investigator: Prof. J. Ugalde*, Government of the Basque Country, SAIOTEK program, 35000.00 €.
Project development
- 2004 – 2007 **Aplicaciones de la Química Cuántica a problemas Químicos seleccionados**, *Principal Investigator: Prof. J. Ugalde*, Spanish Education and Science Office (MEC), CTQ2004–04738.
Project development

Organization of Events

- September 25-30, 2016 **DYNAPEUTICS International Summer School**, *University of the Basque Country (UPV/EHU)*, Donostia, Spain.
Co-organizer

Languages

Basque	Native
Spanish	Native
English	High level
Italian	Intermediate level
French	Basic level

Computer skills

Computational Chemistry Software:	Gromacs, Amber, Charmm, ChemShell, CPMD, CP2K, NWChem, Gaussian, Turbomole, Jaguar, Schrodinger.
Operating Systems:	Linux, Windows, Unix.
Visualization Programs:	VMD, PyMOL, Chimera, Molden, Maestro.

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Publications

Last actualization date: February, 2016

N. Total Cites: 108; **N. Articles:** 11; **Cites/Article:** 9.8; **h-index:** 6

- Authors:** R. Grande-Aztatzi, E. Formoso, J. M. Mercero, J. Matxain, S. J. Grabowski and J. M. Ugalde
Title: Structural and Optical Properties of the Naked and Passivated Al₅Au₅ Bimetallic Nanoluster
Journal: J. Chem. Phys. (2016) **DOI:** 10.1063/1.4943129
ISSN: 0021-9606 **Impact factor:** 2.952 (2014) **Cites:** 0
Category: Physics, Atomic, Molecular & Chemical **Quartile:** Q1
- Authors:** R. Grande-Aztatzi, E. Formoso, J. I. Mujika, J. M. Ugalde and X. Lopez
Title: Phosphorylation Promotes Al(III) Binding to Proteins: GEGEGSGG as a case study
Journal: Phys. Chem. Chem. Phys. (2016) 18, 7197-7202 **DOI:** 10.1039/C5CP06379E
ISSN: 1463-9076 **Impact factor:** 4.493 (2014) **Cites:** 0
Category: Physical Chemistry **Quartile:** Q1
- Authors:** E. Formoso, J. I. Mujika, S. J. Grabowski and X. Lopez
Title: Aluminum and its effect in the equilibrium between folded/unfolded conformation of NADH
Journal: J. Inorg. Biochem. 152, 139-146 (2015) **DOI:** 10.1016/j.jinorgbio.2015.08.017
ISSN: 0162-0134 **Impact factor:** 3.444 (2014) **Cites:** 1
Category: Biochemistry & Molecular biology **Quartile:** Q2
- Authors:** N. B. Luque, J. I. Mujika, E. Formoso and X. Lopez
Title: Aluminum interaction with 2-3-diphosphoglyceric acid. A computational study
Journal: RSC Adv. 5, 63874 (2015) **DOI:** 10.1039/C5RA06796K
ISSN: 2046-2069 **Impact factor:** 3.840 (2014) **Cites:** 2
Category: Multidisciplinary Chemistry **Quartile:** Q1
- Authors:** E. Formoso, V. Limongelli and M. Parrinello
Title: Energetics and Structural Characterization of the large-scale Functional Motion of Adenylate Kinase
Journal: Sci. Rep. 5, 8425 (2015) **DOI:** 10.1038/srep08425
ISSN: 2045-2322 **Impact factor:** 5.078 (2013) **Cites:** 6
Category: Multidisciplinary Sciences **Quartile:** Q1
- Authors:** E. Formoso, J. M. Matxain, X. Lopez and D. York
Title: Molecular Dynamics Simulation of Bovine Pancreatic Ribonuclease A-CpA and Transition State-like Complexes
Journal: J. Phys. Chem. B 114, 7371-7382 (2010) **DOI:** 10.1021/jp909004y
ISSN: 1520-6106 **Impact factor:** 3.603 (2010) **Cites:** 14

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Category: Physical Chemistry

Quartile: Q1

7. **Authors:** J.M. Matxain, E. Formoso, J. M. Mercero, M. Piris, X. Lopez and J. M. Ugalde
Title: Magnetic Endohedral Transition-Metal-Doped Semiconducting-Nanoclusters
Journal: Chem. Eur. J 14, 8547-8554 (2008) **DOI:** 10.1002/chem.200800376
ISSN: 0947-6539 **Impact factor:** 5.454 (2008) **Cites:** 6
Category: Multidisciplinary Chemistry **Quartile:** Q1

8. **Authors:** J.M. Matxain, M. Piris, E. Formoso, J. M. Mercero, X. Lopez and J. M. Ugalde
Title: Endohedral Stannasphenes: Mn@Sn₁₂ and its dimer. Ferromagnetic or Antiferromagnetic?
Journal: Chem. Phys. Chem. 8, 2096-2099 (2007) **DOI:** 10.1002/cphc.200700428
ISSN: 1439-4235 **Impact factor:** 3.502 (2007) **Cites:** 17
Category: Physical Chemistry **Quartile:** Q1

9. **Authors:** J.M. Matxain, L. A. Eriksson, E. Formoso, M. Piris, and J. M. Ugalde
Title: Endohedral X@Zn_iS_i^q compounds: X=Li,Na,K,F,Cl,Br, q=-1,0,1 and i=4-16
Journal: J. Phys. Chem. C, 111, 3560-3565 (2007) **DOI:** 10.1021/jp0668697
ISSN: 1932-7447 **Impact factor:** 3.396 (2008) **Cites:** 11
Category: Physical Chemistry **Quartile:** Q1

10. **Authors:** J.I. Mujika, E. Formoso, J.M. Mercero, and X. Lopez
Title: Reaction Mechanism of the Acidic Hydrolysis of Highly Twisted Amids: Rate Acceleration Caused by the Twist of the Amide Bond
Journal: J. Phys. Chem. B, 110, 1500-1511 (2006) **DOI:** 10.1021/jp0604037
ISSN: 1520-6106 **Impact factor:** 4.115 (2006) **Cites:** 23
Category: Physical Chemistry **Quartile:** Q1

11. **Authors:** J.M. Mercero, E. Formoso, J.M. Matxain, L. A. Eriksson, and J.M. Ugalde
Title: Sandwich complexes based on the "all-metal" Al₄⁻² aromatic rings.
Journal: Chem. Eur. J. 12, 4495-4502 (2006) **DOI:** 10.1002/chem.200600106
ISSN: 0947-6539 **Impact factor:** 5.015 (2006) **Cites:** 28
Category: Multidisciplinary Chemistry **Quartile:** Q1

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