

CV Date	12/01/2022
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Part A. PERSONAL INFORMATION

First Name	Hegoi		
Family Name	Manzano Moro		
Sex	Male	Date of Birth	20/05/1981
ID number Social Security, Passport	45662626J		
URL Web	https://sites.google.com/view/hegoimanzano		
Email Address	hegoi.manzano@ehu.eus		
Open Researcher and Contributor ID (ORCID)	0000-0001-7992-2718		

A.1. Current position

Job Title	Profesor Agregado		
Starting date	2021		
Institution	Universidad del País Vasco		
Department / Centre	Física / Facultad de Ciencia y Tecnología		
Country		Phone Number	
Keywords	Description; Defects; Mechanical properties; Structural phase transition; Structure; Thermodynamics		

A.2. Previous positions (Research Career breaks included)

Period	Job Title / Name of Employer / Country
2017 - 2021	Profesor Adjunto / Universidad del País Vasco
2015 - 2017	Profesor Laboral Interino / Universidad del País Vasco
2014 - 2015	Investigador Doctor Juan de la Cierva / Universidad del País Vasco
2013 - 2013	Personal Investigador Contratado / Universidad del País Vasco
2012 - 2012	Investigador Doctor del Gobierno Vasco / Universidad del País Vasco
2010 - 2011	Postdoctoral Fellow / Massachusetts Institute of Technology (USA).
2005 - 2009	Becario predoctoral / Labein-Tecnalia

A.3. Education

Degree/Master/PhD	University / Country	Year
Química	Universidad del País Vasco	2009
Estudios Avanzados en Química de Materiales y Superficies	Universidad del País Vasco	2007
Licenciado en Ciencias Químicas Especialidad Química Fundamental Opción Química Física	Universidad del País Vasco	2005

Part B. CV SUMMARY

Hegoi Manzano obtained his Degree in Physical Chemistry in 2005 at the University of the Basque Country UPV/EHU. He did an industrial PhD in TECNALIA, a R+D company sited in the Basque Country (Spain), obtaining the PhD in Chemistry from the University of the Basque Country in 2009, with a thesis on "Atomistic modelling of cement-related materials". Right after obtaining the PhD, he won a DKR postdoctoral grant from the Basque Country Government and he moved to MIT in January 2010, where he stayed 2 years as a postdoc. He continued his studies in cement-based materials, working on reactive force field development and its application. In 2012 he moved back to Spain, to the University of the Basque Country, where he occupied several postdoc research positions (DKR, PIC, and Juan de la Cierva) until 2015.

Then, he obtained a position as "Profesor Laboral interino" and "Profesor Adjunto" (Assistant Professor) at the Physics Department of the UPV/EHU until 2021, when he obtained his permanent position as "Profesor Agregado" (Associated Professor).

Scientific-technical achievements:

Hegoi Manzano leads a small group at the UPV/EHU focused on atomic and mesoscale modelling of cement-related materials. He has been working on this topic his PhD thesis, the first in the field. In his group they use a large number of different atomic and mesoscale methodologies (Density Functional Theory, Molecular Dynamics, Evolutionary Algorithms, Kinetic Monte Carlo) to investigate each problem with the most appropriate technique and from multiple perspectives. They focus on the dissolution of minerals and the its application to cement, as well as the nucleation and properties of the C-S-H gel. A summary of his achievements is listed below:

- 61 publications in JCR journals (32 as first or corresponding author, 37 Q1) including high IF journals (JACS, Adv. Materials, Adv. Functional Materials, Adv. Energy Materials)
- 2 book chapters
- h-index 27, total times cited 2951 (data Google Scholar)
- 32 contributions in scientific meetings (4 invited, 22 communications, and 6 posters)
- Participation in 21 funded research projects (2 as IP) and 5 private research contract (4 as IP)
- 2 years MIT (Cambridge, USA) and short stays from 2 weeks to 1 month in Newcastle U (UK), University of the British Columbia (Canada), Bonn U y Dresden TU (Germany)

Capabilities of training young researchers and evaluation committees:

At the UPV/EHU Hegoi Manzano teaches Experimental Techniques in Physics and Statistical Physics in the Physics degree. He has a close contact with students, always trying to convey them his interest in science. As a result, he has supervise students at every stage. He has also participate in the organisation of several scientific events, and is an active reviewer of scientific publications and EU projects.

- Supervision of 17 Undergraduate Students, 6 M.Sc., and 5 Ph.D. students (2 finished)
- Member of 2 organizing committees of scientific events, 3 hands-on workshops
- Evaluation of 2 EU Prace projects (22th and 23rd calls) and a project from the German Research Foundation (FU991/2-1)
- > 70 reviews for JCR journals since 2016.
- 4 Ph.D. evaluation tribunals

Grants and awards:

- Juan de la Cierva from the Spanish Government
- DKR Postdoctoral Grant from the Basque Country Government
- Iñaki Goenaga PhD grant from Fundación Centros Tecnológicos

Part C. RELEVANT ACCOMPLISHMENTS

C.1. Most important publications in national or international peer-reviewed journals, books and conferences

AC: corresponding author. (n° x / n° y): position / total authors. If applicable, indicate the number of citations

- 1 **Scientific paper.** de Larramendi, Idoia Ruiz; Lozano, Iñigo; Enterría, Marina; et al; others. 2021. Unveiling the Role of Tetrabutylammonium and Cesium Bulky Cations in Enhancing Na-O₂ Battery Performance *Advanced Energy Materials*. pp.2102834-2102834.
- 2 **Scientific paper.** Martín, Pablo; Manzano, Hegoi; Dolado, Jorge S. 2019. Mechanisms and Dynamics of Mineral Dissolution: A New Kinetic Monte Carlo Model *Advanced Theory and Simulations*. 2-10, pp.1900114-1900114.
- 3 **Scientific paper.** Zhou, Yang; Orozco, Carlos A; Duque-Redondo, Eduardo; Manzano, Hegoi; Geng, Guoqing; Feng, Pan; Monteiro, Paulo JM; Miao, Changwen. 2019. Modification of poly (ethylene glycol) on the microstructure and mechanical properties of calcium silicate hydrates *Cement and Concrete Research*. Pergamon. 115, pp.20-30.
- 4 **Scientific paper.** Duque-Redondo, E.; Kazuo, Y.; López-Arbeloa, I.; Manzano, H. 2018. Cs-137 immobilization in C-S-H gel nanopores *Physical Chemistry Chemical Physics*. 20-14. ISSN 14639076.
- 5 **Scientific paper.** Zhou, Y.; Hou, D.; Manzano, H.; Orozco, C.A.; Geng, G.; Monteiro, P.J.M.; Liu, J.(3/7). 2017. Interfacial Connection Mechanisms in Calcium-Silicate-Hydrates/Polymer Nanocomposites: A Molecular Dynamics Study *ACS Applied Materials and Interfaces*. 9-46, pp.41014-41025. ISSN 19448252.
- 6 **Scientific paper.** Mishra, R.K.; Mohamed, A.K.; Geissbühler, D.; et al; Manzano, H.; Bowen, P.(4/15). 2017. cemff: A force field database for cementitious materials including validations, applications and opportunities *Cement and Concrete Research*. ISSN 00088846.
- 7 **Scientific paper.** Hegoi Manzano; Ixone Esnal; Tamara Marqués-Matesanz; et al; Jose Luis Chiara. (1/10). 2016. Unprecedented J?Aggregated Dyes in Pure Organic Solvents *Advanced Functional Materials*. Wiley-VCH. 26-16, pp.2756-2769. ISSN 1616-301X. <https://doi.org/10.1002/adfm.201505051>
- 8 **Scientific paper.** Manzano, H.; Durgun, E.; López Arbeloa, I.; Grossman, J.C. 2015. Insight on tricalcium silicate hydration and dissolution mechanism from molecular simulations *ACS Applied Materials and Interfaces*. 7-27, pp.14726-14733. ISSN 1944-8244.
- 9 Duque-Redondo, Eduardo; Yamada, Kazuo; Manzano, Hegoi. 2021. Cs retention and diffusion in C-S-H at different Ca/Si ratio *CEMENT AND CONCRETE RESEARCH*. 140. ISSN 0008-8846. WOS (3) <https://doi.org/10.1016/j.cemconres.2020.106294>
- 10 Dupuis, Romain; Moon, Juhyuk; Jeong, Yeonung; et al; Dolado, Jorge S. 2021. Normal and anomalous self-healing mechanism of crystalline calcium silicate hydrates *CEMENT AND CONCRETE RESEARCH*. 142. ISSN 0008-8846. <https://doi.org/10.1016/j.cemconres.2021.106356>

C.2. Conferences and meetings

- 1 Dissolution mechanism of C₃S and CaO. The 15th International Congress on the Chemistry of Cement. Praga TU. 2019.
- 2 Distinctive Diffusion Regimes of Organic Molecules in Clays. XVI International CLay Conference. Universidad de Granada. 2017. Spain.
- 3 Hegoi Manzano Moro. Molecular simulation of mineral dissolution. Atomistic Simulation in Cementitious Systems "Cement force field database". Nanocem. 2018. Switzerland. Participatory - invited/keynote talk. Workshop.
- 4 Hegoi Manzano. Hydration of Alite from Molecular Simulation. The 14th International Congress on the Chemistry of Cement. Chinese Ceramic Society. 2015. China. Participatory - oral communication. Conference.
- 5 Hegoi Manzano. The Role of Water on C-S-H Gel Shear Strength Studied by Molecular Dynamics Simulations. CONCREEP 10. American Society of Civil Engineers. 2015. Austria. Participatory - oral communication. Conference.
- 6 Feng Li; Xiaodong Shen; Iñigo Lopez-Arbeloa; Hegoi Manzano; Yanhua Guo; Qianqian Wang. First-principles study of water adsorption and dissociation on α -C₂S (100) surface. RILEM International Symposium on Concrete Modeling-CONMOD 2014. Tsinghua University - RILEM. 2014. China.

- 7 Hegoi Manzano. New insight of Mineral Hydration from Reactive force field molecular dynamics. Multiscale Materials under the nano scope 2014 workshop. Donostia International Physics Center. 2014. Spain. Participatory - invited/keynote talk. Workshop.
- 8 Hegoi Manzano. Overview of ReaxFF and its application to material hydration. Colloquium of the German Chemical Society. German Chemical Society. 2014. Germany. Participatory - invited/keynote talk. Seminar.
- 9 Hegoi Manzano. Ultraviolet/visible dual absorption by single BODIPY dye confined in LTL zeolite nano channels. VI Jornadas de Jóvenes investigadores en Física atómica y molecular. Universidad del País Vasco. 2014. Spain. Participatory - oral communication. Workshop.

C.3. Research projects and contracts

- 1 **Project.** Simulación computacional y caracterización fotofísica avanzada de biosondas moleculares inteligentes. Ministerio de Ciencia e Innovación. Jorge Bañuelos Prieto. (Universidad del País Vasco). 01/01/2021-31/12/2023. 114.950 €.
- 2 **Project.** Síntesis de nanotransportadores y caracterización fotofísica asistida computacionalmente de colorantes y materiales multifuncionales para aplicaciones biofóticas. Ministerio de Ciencia e Innovación. Investigación. (Universidad del País Vasco). 01/01/2018-31/12/2020. 108.900 €.
- 3 **Project.** Baskrete Joint Reserach LAB. Universidad del País Vasco. (Universidad del País Vasco). 01/01/2018-31/12/2018. 9.000 €.
- 4 **Project.** Síntesis, simulación atomística y caracterización fotofísica de materiales nanoestructurados híbridos para aplicaciones fotónicas y biofóticas. Ministerio de Ciencia e Innovación. Investigación. Iñigo López Arbeloa. (Universidad del País Vasco). 01/01/2015-31/12/2017. 101.640 €. Team member.
- 5 **Project.** Advanced Manufacturing of Nanomaterials by supercritical FLuid Technology. Gobierno Vasco. Jorge Sanchez Dolado. (Universidad del País Vasco). 01/01/2016-31/07/2017. 33.112 €.
- 6 **Project.** ETORTEK14/04, ETORTEK 2014: Consolidación de los grupos de nanobiomecánica, teoría, nanomateriales y nanoimagen del CIC nanogune, y desarrollo de investigación tecnológico en el ámbito de la corrosión y la incrustación. ETORTEK. Hegoi Manzano. (Universidad del País Vasco). 01/01/2014-31/12/2015. 39.929 €. Co-ordinator.
- 7 **Contract.** MOLECULAR DYNAMIC SIMULATION OF THE SELECTIVITY COEFFICIENT OF CS AGAINST NA IN CALCIUM ALUMINOSILICAT E HYDRATES (C- A-S-H) WITH VARIABLE PORE SIZE National Institute of Environmental Studies. Hegoi Manzano Moro. (Universidad del País Vasco). 01/02/2020-01/08/2020. 8.094,19 €.
- 8 **Contract.** Simulación por Dinámica Molecular de adsorción competitiva de Cs y Na en C-A-S-H y Distribución deNa y agua en geopolímeros National Institute of Environmental Studies. Hegoi Manzano Moro. (Universidad del País Vasco). 01/02/2019-01/11/2019. 19.622 €.
- 9 **Contract.** Additional analysis on the former contract work ¿MD calculation of the interaction between Cs and cement hydrates relating Cs transfer in concrete used for disposal of radio-nuclide contaminated wastes National Institute of Environmental Studies. Hegoi Manzano Moro. (Universidad del País Vasco). 31/05/2018-30/10/2018. 7.477 €.
- 10 **Contract.** MD simulation of the interaction between Cs and cement hydrates relating Cs transfer in concrete used for disposal of radio-nuclide contaminated wastes National Institute of Environmental Studies. Hegoi Manzano Moro. (Universidad del País Vasco). 01/10/2015-01/10/2016. 17.400 €.