

CURRICULUM VITAE ABREVIADO (CVA)

IMPORTANT – The Curriculum Vitae cannot exceed 4 pages. Instructions to fill this document are available in the website.

Part A. PERSONAL INFORMATION

First name	Antonio M.		
Family name	Márquez Cruz	Date	4/07/2023
Open Researcher and Contributor ID (ORCID) (*)	0000-0001-6699-064X		

(*) Mandatory

A.1. Current position

Position	Full Professor		
Initial date	21/12/2017		
Institution	Universidad de Sevilla		
Department/Center	Department of Physical Chemistry		
Country	Spain	Teleph. number	955421002
Key words	Materials simulations, DFT, heterogeneous catalysis		

A.2. Previous positions (research activity interruptions, indicate total months)

Period	Position/Institution/Country/Interruption cause
1987-1990	PhD Student (Becario FPI)/University of Sevilla/Spain
1991-1992	Postdoctoral Scientist/IBM Corporation/USA
1992-1995	Postdoctoral Scientist/Univ. of Sevilla/Spain
1995-2000	Associated professor/Univ. of Sevilla/Spain
2000-2017	University professor/Univ. of Sevilla/Spain

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
Licensed, Chemistry	University of Sevilla, Spain	1986
PhD, Chemistry	University of Sevilla, Spain	1991

(Include all the necessary rows)

Part B. CV SUMMARY (max. 5000 characters, including spaces)

PhD in Chemistry in 1991 from the University of Sevilla with full honors. Worked in 1991-1992 at the "Chemistry Applications Management" Department of IBM Kingston as a postdoctoral researcher with Dr. Michel Dupuis. My postdoctoral research was focused on the implementation of efficient algorithms for post-SCF methods that could be applied to large molecular systems. Back to the University of Sevilla I focused my research on the implementation of parallel algorithms in Quantum Chemistry methods and started to study the structure and reactivity on solid heterogeneous catalysts using cluster models, in strong collaboration with the group of Prof. Francesc Illas (UB) and Prof. Gianfranco Pacchioni (Univ. Milano-Bicocca). In relation with these interests, I was invited in 1999 to the Univ. of Barcelona under the program "Access to Supercomputing Facilities for European Researchers". In 2000, I became professor of Physical Chemistry and since then his investigations centered in the study, by means of theoretical models, of the structure and reactivity of solid systems and surfaces with emphasis on diverse heterogeneous catalysis problems. In the research projects related to this topic I continued my collaboration with Prof. Illas (UB) and also started a cooperation with the experimental catalysis group of prof. José Antonio Odriozola (USE) and also with prof. Richard Lambert, (University of Cambridge). More recently, I have initiated a new line on our group focused on the development of computational methods including Machine Learning algorithms for the study of the thermoelectric properties of materials in large chemical spaces. In this research line we have a strong collaboration with Prof. Ricardo Grau-



Crespo (Univ. of Reading, UK). My expertise covers theoretical methods based on quantum-mechanics theory and statistical mechanics, using wavefunction and DFT methods, and molecular dynamics simulations.

Currently I am PI of two research projects (TED2021-130874B and PID2019-106871GB-I00) that aim to the study of the thermoelectric properties of materials, including Machine Learning methodology to address both the complexity of the calculation of some of these properties and the exploration of large chemical spaces. In the last ten years I also have participated as senior researcher in three other projects (CTQ2015-64669-P, MAT2012-31526, and P2-FQM-1595) related to the study of the properties of oxide-supported metal and chalcogenide nanoparticles. In these projects we examined the catalytic properties and/or the electronic structures of these systems in relation to their use as components of third generation solar cells absorbers. Two of the PhD theses that I have supervised were results of the research performed in these projects.

Moreover, I also have been involved in two technological development projects in collaboration with the Repsol Technology Lab (included in the CVA). In these projects the expertise of our group in the study of the reactivity of chemical systems allowed us to understand a complex process of catalytic epoxidation and the practical difficulties encountered by Repsol in its implementation. The second project aimed to develop models and methodology to calculate and rationalize the liquid-liquid and solid-liquid interactions in relation to the problem of crude extraction in oil reservoirs.

In relation with my duties in superior education, I have been regularly in charge and coordinator of undergraduate Physical Chemistry courses for about 20 years. Simultaneously he has been teaching postgraduate (Doctorate and Master) courses related to Molecular Modelling and Electronic Structure and Properties of Solids and Surfaces being coordinator of the latter at the Master in Theoretical Chemistry and Computational Chemistry (TCCM), recognized as Erasmus Mundus Joint Master Degree under the Erasmus+ Program.

I regularly act as reviewer of research papers for high-quality journals like J. Phys. Chem.; J. Am. Chem. Soc.; Phys. Rev. Lett.; Phys. Rev. B; Phys. Rev. Mat.; Surf. Sci.; Phys. Chem. Chem. Phys.; Scientific Reports; Physica B; Appl. Surf. Sci.; ACS Appl. Mater. Interfaces; Comput. Theor. Chem. I also assist regularly to the evaluation of projects to the MICINN and FONDECYT.

Summary of scientific production:

- Number of publications: 97 (Scopus), ~70% in Q1 journals.
- Total citations: 2214 (Scopus), 2923 (Google Scholar), with 6 papers with more than 100 citations and 16 with more than 50 citations (Google Scholar).
- h-index: 27 (Scopus), 32 (Google Scholar)

Part C. RELEVANT MERITS (sorted by typology)

C.1. Publications (see instructions)

1. E. J. Blancas, J. J. Plata, J. Santana, F. Lemus-Prieto, A. M. Márquez, J. Fdez Sanz Unraveling the role of chemical composition in the lattice thermal conductivity of oxychalcogenides as thermoelectric materials. *J. Mater. Chem. A*, **2022**, *10*, 19941-19952 (Prof. Plata - Themed Collection: J. Mater Chem. A, Emerging Investigators)
2. J. J. Plata, V. Posligua, A. M. Márquez, J. Fdez. Sanz, R. Grau-Crespo. Charting the Lattice Thermal Conductivities of I–III–VI₂ Chalcopyrite Semiconductors. *Chem. Mater.* **2022**, *34*, 2833-2841 (Main Cover of the issue).
3. J. J. Plata, P. Nath, J. Fdez. Sanz, A. M. Márquez. In silico modeling of inorganic thermoelectric materials. In *Comprehensive Inorganic Chemistry III*. Elsevier. 2022
4. J. Amaya Suárez, J.J. Plata, A.M. Márquez, J. Fdez Sanz. Catalytic Activity of PtCu intermetallic compound for CO oxidation: A theoretical insight. *Cat. Today* **2022**, *383*, 339-344.



5. P. Nath, J.J. Plata, J. Santana, E.J. Blancas, A.M. Márquez, J. Fdez Sanz. High-Throughput Screening of the Thermoelastic Properties of Ultrahigh-Temperature Ceramics. *ACS Appl. Mater. Interfaces*, **2021**, *13*, 29843-29857.
6. J.J. Plata, A.M. Márquez, S. Cuesta-López, J. Fdez Sanz. Connecting Experimental Synthetic Variables with the Microstructure and Electronic Properties of Doped Ferroelectric Oxides Using High-Throughput Frameworks. *Acta Materialia*, **2021**, *204*, 116466.
7. J.J. Plata, J. Amaya Suárez, S. Cuesta-López, A.M. Márquez, J. Fdez Sanz. Photosensitizing thin-film ferroelectric oxides using materials database and high-throughput calculations. *J. Mater. Chem. A* **2019**, *7*, 27323-27333.
8. G. Kyriakou, A.M. Márquez, J.P. Holgado, M.J. Taylor, A.E.H. Wheatley, J.P. Metha, J. Fdez Sanz, S.K. Beaumont, R.M. Lambert. A comprehensive experimental and theoretical study of the CO+NO reaction catalyzed by Au/Ni nanoparticles. *ACS Catal.* **2019**, *9*, 9419-9429.
9. N. Orozco, G. Kyriakou, S.K. Beaumont, J. Fdez. Sanz, J.P. Holgado, M.J. Taylor, J.P. Espinós, A.M. Márquez, D.J. Watson, A.R. González-Elipe, R.M. Lambert. Critical role of oxygen in silver-catalyzed Glaser-Hay coupling on Ag (100) in vacuum and solution on Ag particles. *ACS Catal.* **2017**, *7*, 3113-3120.
10. J.J. Plata, L.C. Pacheco, E.R. Remesal, M.O. Masa, L. Vega, A.M. Márquez, J.A. Odriozola, J. Fdez Sanz. Analysis of the variables that modify the robustness of Ti-SiO₂ catalysts for alkene epoxidation: Role of silylation, deactivation and potential solutions. *Mol. Catal.* **2018**, *459*, 55-60.
11. J.J. Plata, A. M. Márquez, and J. Fdez. Sanz. Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. *Chem. Mater.* **2014**, *26*, 3385- 3390.
12. J.J. Plata, A.M. Márquez, J. Fdez-Sanz. Electron mobility via polaron hopping in bulk ceria: a first principles-study. *J. Phys. Chem. C.* **2013**, *117*, 14502-14509.

C.2. Congress, indicating the modality of their participation (invited conference, oral presentation, poster)

1. **12th Congress on electronic Structure: Principles and Applications**. July 2018 (Vigo, Spain) Plenary talk "Exploring the role of chemical composition in the lattice thermal conductivity of thermoelectric materials assisted by machine learning." J.J. Plata, E. J. Blancas, J. Santana, A.M. Márquez, J. Fdez Sanz.
2. **50 Years of Quantum Chemistry in Strasbourg**, Nov 2019 (Strasbourg, France). Plenary talk: "A Combinatorial approach for the study of disordered photosensitized ferroelectric materials". A.M. Márquez, J.J. Plata, J. Amaya Suárez, and J. Fdez Sanz.
3. **14th International Conference on Materials Chemistry**, Jul 2019 (Birmingham, UK). Plenary talk: "Combining materials databases and high-throughput computing for the discovery of new photo-sensitized ferroelectric materials". J.J. Plata, J. Amaya Suárez, A.M. Márquez, J. Fdez Sanz.
4. **The 17th International Conference on the Formation of Semiconductor Interfaces**, Jun 2019 (Shanghai, China). Oral communication: "Design of Epitaxially Grown Ferroelectric Perovskite Photosensitizers from High-Throughput Computations". J.J. Plata, A.M. Márquez, J. Fdez Sanz.
5. **3rd International Conference on Applied Surface Science**. Jun 2019 (Pisa, Italy). Oral communication: "High-throughput search of substrates for the discovery of new epitaxy photo-sensitized ferroelectric structures". J. Amaya Suárez, J.J. Plata, A.M. Márquez, J. Fdez Sanz.
6. **3rd International Conference on Applied Surface Science**. Jun 2019 (Pisa, Italy). Oral communication: "A Combinatorial approach for the study of disordered photosensitized ferroelectric materials". A.M. Márquez, J.J. Plata, J. Amaya Suárez, and J. Fdez Sanz.
7. **11th International Workshop on Oxide Surfaces (IWOX-XI)**, Jan 2018 (Sierra Nevada, Spain). Plenary talk: "Structure of the SiO₂/brine/oil interface. A Molecular Perspective Based on Molecular Dynamics Calculations". J.J. Plata, J. Amaya Suárez, A.M. Márquez, J. Fdez Sanz.



8. **11th International Workshop on Oxide Surfaces (IWOX-XI)**, Jan 2018 (Sierra Nevada, Spain). Plenary talk: "*Sensitizing Epitaxial Structures for Sunlight Harvesting: A High-throughput Approach*". J.J. Plata, J. Amaya Suárez, A.M. Márquez, J. Fdez Sanz.
9. **Workshop on Quantum Systems in Chemistry, Physics, and Biology**, Dec 2013 (Paraty, Rio de Janeiro, Brazil). Oral communication: "*Charge transport at CeO₂ Interfaces: Electron Mobility and Oxygen Ion Migration*". J. Fdez Sanz, J.J. Plata, A.M. Márquez.

C.3. Research projects.

As IP.

1. Ref. PID2019-106871GB-I00. Title: Diseño y modelización computacional de materiales termoeléctricos basados en calcogenuros y oxicalcogenuros metálicos. 1/07/2020 – 31/05/2023. Ministerio de Ciencia e Innovación. Grant: 54 450 €. Status: finished.
2. Ref. TED2021-130874B-I00. Title: Búsqueda y optimización de la eficiencia termoeléctrica de escuteruditas usando bases de datos, entornos de alto rendimiento, simulaciones atomísticas y aprendizaje automático. 1/12/2022-ongoing. Ministerio de Ciencia e Innovación. Grant: 160 000 €. Status: ongoing.

As participant.

1. Ref. CTQ2015-64669-P. Title: Diseño computacional de Catalizadores Avanzados: nanopartículas metálicas soportadas sobre óxidos metálicos mixtos. IP: Javier Fernández Sanz. 1/1/2016-31/12/2019. MINECO. Grant: 61 589 €. Status: finished.
2. Ref. MAT2012-31526. Title: Simulación de Catalizadores: Nanopartículas de Metales y Óxidos Metálicos Depositadas en Soporte: Estructura, Propiedades Electrónicas y Actividad Catalítica. IP: Javier Fernández Sanz. 1/1/2013-31/12/2015. MINECO. Grant: 55 000 €. Status: finished.
3. Ref. P12-FQM-1595. Title: Celdas solares con sensibilizador: Propiedades electrónicas de nanoestructuras de sulfuros metálicos utilizados como captorees de energía (QDSC). IP: J. Fernández Sanz. 31/1/2014-16/2/2019. Junta de Andalucía. Grant: 150 644 €. Status: finished.
4. Sensitized solar cells: Computational simulations of the electrolyte/semiconductor interphase Funded by: Junta de Andalucía, Excellence Program, Project P08-FQM-03661. 3-01-2009 to 13-01-2013 Grant: 151.323 €.
5. Funcionalización superficial de materiales para aplicaciones de alto valor añadido (FUNCOAT) Funded by: MICINN, Consolider-Ingenio, Project: CSD2008-00023. 25/12/2008 to 15/12/2014. Grant (USE): 199.672 €.

C.4. Contracts, technological or transfer merits.

1. Title: Aplicación de la Química Computacional a procesos catalíticos de epoxidación. (1735/0638). REPSOL S. A. 20/12/2012-30/09/2013. Amount: 38.500 € IP: J. Fernández Sanz.
2. Title: Estudio computacional de la interacción entre un material silíceo y dos fluidos inmiscibles (2264/0638). REPSOL S.A. 1/7/2014-30/11/2015. Amount: 100.000 € IP: J.Fernández Sanz.