



CURRICULUM VITAE (CVA)

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

Part A. PERSONAL INFORMATION

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|----------------|------------|
| CV date | 17/02/2023 |
|----------------|------------|

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|---|-----------------------------------|----------------------------|--|
| First name | José Ignacio | | |
| Family name | Martínez | | |
| Gender (*) | Male | Birth date (dd/mm/yyyy) | 22/06/1979 |
| Social Security, Passport, ID number | 12407687S | | |
| e-mail | Joseignacio.martinez@icmm.csic.es | | URL Web https://wp.icmm.csic.es/esisna/jose-ignacio-martinez/ |
| Open Research and Contributor ID (ORCID)(*) | 0000-0002-2086-8603 | | |

(*) *Mandatory*

A.1. Current position

| | | | |
|--------------------|---|-------------|-----------|
| Position | Tenured CSIC Scientist | | |
| Initial date | 31/07/2020 | | |
| Institution | Consejo Superior de Investigaciones Científicas | | |
| Departament/Center | Instituto de Ciencia de Materiales de Madrid | | |
| Country | Spain | Tel. number | 913349095 |
| Key words | Surface Science, 2D Materials, Clusters, Nanoparticles, DFT, STM, Nanostructured Materials, Computational Physico-chemistry | | |

A.2. Previous positions (research activity interruptions, art. 45.2.c))

| Period | Position/Institution/Country/Interruption cause |
|--------------|---|
| 2003-2007 | FPI Fellow at Facultad de Ciencias (UVA), Spain |
| 2007-2009 | Postdoctoral researcher at CAMD-DTU, Denmark |
| 2009-2013 | Postdoctoral researcher at Facultad de Ciencias (UAM), Spain (including a JdC Fellowship) |
| 2013-2020 | Postdoctoral researcher at ICMM-CSIC, Spain (including JaeDOC and RyC Fellowships) |
| 2020-present | Tenured CSIC Scientist |

A.3. Education

| | | |
|----------------------------|----------------------------------|------|
| PhD, Licensed, Graduate | University/Country | Year |
| PhD in Theoretical Physics | University of Valladolid / Spain | 2007 |
| Advanced Studies Diploma | University of Valladolid / Spain | 2004 |
| Degree in Physics | University of Valladolid / Spain | 2002 |

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

Tenured CSIC Scientist at the ICMM-CSIC (Madrid) since 2020. Bachelor in Physics at University of Valladolid (UVA), 2002. PhD summa cum laude in Physics (J. A. Alonso's group):

catalytic, mechanical and photoresponse properties of small metal and organometallic clusters) at UVA, 2007. Post-doctoral positions in prestigious Research Groups of Catalysis and Surface Science: FP7 post-doc at CAMD-DTU (Denmark), 2007-2009 (J. K. Norskov's group: stability and catalytic properties of inexpensive catalysts); FP7 and JdC post-docs at the Autonomous University of Madrid (UAM), 2009-2013 (F. Flores' group: organic/inorganic interfaces). CSIC-JaeDoc scientist (2013-2015) at the ICMM-CSIC (Madrid) carrying out first-principles simulations of low-dimensional systems to guide Surface Science experiments. Afterwards, I held a contracted scientist FC3 position associated to the ERC-Synergy NANOCOSMOS Project (15 M€) at ICMM-CSIC, devoted to the first-principles-based simulation of the interaction of small nanoparticles with gas at the circumstellar environment. Ramón y Cajal fellowship (2017-2020) in the area of "Physics and Space Science" at ICMM/CSIC. Currently, Head of the Dept. Low-dimensional Systems in the ICMM-CSIC.

During my research career I have covered the study of nanostructured functional materials from a highly interdisciplinary approach, involving chemistry, physics, and computational science, towards the guidance of multidisciplinary material science experimentalists on the basis of an efficient, fast and trustable theoretical pre-filtering of materials across dimensionality and their nanostructured versions on demand of the specific targeted functionalities. My researching interests have been focused on three main branches. The first one is the "*Theory and First-principles Simulation of Low-dimensional Functional Materials*" towards: i) the conceptual development of theoretical tools and models to understand the behavior of nanostructured and low-dimensional materials and surfaces in nature, ii) the characterization of structural, chemical reactivity and spectroscopic properties of low-dimensional materials with enhanced and emerging properties regarding targeted functionalities, and iii) the development of first-principles theoretical frameworks applied to multidisciplinary fields such as surface physics, computational physics, characterization of nanomaterials (from small clusters/nanoparticles, nanowires/tubes and layered materials, to their extended surfaces), catalysis, physico-chemical modeling and on-surface chemistry. On the other hand, a large part of my investigation has been devoted to the "*In-silico Design and Characterization of Novel Low-dimensional Functional Materials and Processes*", involving **functionalization of graphene and graphitic nanomaterials** (as robust platforms towards the design and development of novel nano-hybrid sensors), **TMDCs nanostructures** for hydrogen storage purposes, on-surface-driven formation of organic low-dimensional nanostructures, organic/metal (O-M) and organic/metal-oxide (O-MO) interfaces, multi-stimuli responsive 2D-coordination polymers (as electronic, optical and gas-sensing platform), **novel chemical routes and nanomaterials** (thermally-assisted H-induced etching of carbonaceous species) to explain the formation of PAHs in space, **carbonaceous, SiC-based and organometallic clusters** with high interest in astrochemistry and metal nanoparticles (with enhanced optical and catalytic properties), and **advanced functional nanostructured catalysts** (theoretical pre-filtering for their use in fuel/solar cell devices). Finally, all the researching interests and aforementioned lines developed with the main purpose of "*Developing Simple and Predictive First-principles-based Descriptors Across Dimensionality of Materials*" linking and correlating their different structural, intrinsic stability, electronic structure and chemical reactivity properties.

My investigation in these fields is reflected in >140 JCR articles attracting >6500 citations (WoS), granted with 15 artistic journal covers. I am coauthor of 5 book chapters (one in a CRC Handbook of Nanophysics) with 1 national and 1 European patent. Participation in 21 I+D+i projects, (3 FP7 and 1 ERC-Synergy European projects). In 2017 I led as PI and coordinator my first researching project (200.000 €) devoted to the study of functional low-dimensional materials for the development of electrochemical (bio)sensors. Personally, I have attracted > 800.000 € of research funding (leading 6 projects as PI). Supervision of 2 TFG, 1 TFM, 1 PhD student and 1 Postdoc researcher. Since 2015 I belong to the experts-panel of different scientific national agencies: ANEP and AEI (Spain), FWF (Austria) and ANPCyT (Argentina). Participation in technological and knowledge transfer activities with several technological enterprises (Germanos, Nedstack, Samsung Korea), being PI in 2 Technological Assistance

Contracts with Dynasol S.L. Coordinator of a large number of scientific divulgation and "outreach" activities.

Part C. RELEVANT MERITS (*sorted by typology*)

- **Bibliometric Indicators:** (WoS/GoogleScholar) Total citations: 6700/8300; H: 33/37
- **Academic Honors and Awards:** 2007: Extraordinary PhD thesis award (UVA), 2015: Ramón y Cajal Fellowship (Spanish Ministry of Science and Technology)
- **Activity as supervisor:** 2 TFG, 1 TFM, 1 PhD student and 1 Postdoc researcher
- **Teaching:** over 60 ECTS (~500 teaching hours validated by the ANECA) in courses of Physics and Chem. Eng. Degrees. Invited to teach a number of master classes within a Nanotechnology Master Program at CNRS (France). Ad-honorem Professor at UAM since 2013; and accredited Professor (Assistant, Contracted and Private University Professor) by Spanish ANECA
- **Memberships of scientific societies and evaluation committees:** Member of two specialized groups (GEFES and GEFAM) of the Spanish Royal Society of Physics (RSEF). Member of ASEVA. Experts panel of different scientific national agencies: ANEP and AEI (Spain), FWF (Austria) and ANPCyT (Argentina). Member of the scientific committee of the "European Workshop on Epitaxial Graphene and 2D Materials". Frequent referee for the most prestigious scientific editorials (Nature PG, APS, ACS, RSC, Wiley, IOP, Elsevier). PhD. Theses examiner: 5 (3 Madrid / 1 Donostia, Spain) | 1 (Leiden, The Netherlands).
- **Collaborations:** A wide network of national and international collaborations: F. Zamora's (UAM/Spain: 2D Coordination-polymers), M. Gottfried's (University of Marburg/Germany: Organic-oxide Interfaces), M.T.M Koper's (Leiden University/The Netherlands: Theoretical Electrochemistry), R.A. Bartyński's (University of New Jersey: Organometallic Interfaces), A. Zak's (KIT/Israel: Layered Materials: Hydrogen Storage), R. Fasel's (EMPA/Switzerland: On-surface Chemistry). J. Coraux (Neel Inst./France), among others.
- **Facilities:** Setting up of a High-performance Scientific Computing Clusters at the UAM and the ICMM-CSIC (Madrid) with >200 calculation nodes.

C.1. Publications (see instructions)

- *Metal-catalyst-free gas-phase synthesis of long-chain hydrocarbons.* L. Martínez, P. Merino, G. Santoro, J. I. Martínez, J. Ault, A. Mayoral, L. Vázquez, S. Katsanoulis, M. Accolla, A. Dazzi, J. Mathurin, F. Borondics, E. Blázquez-Blázquez, J. E. Quintanilla-López, R. Jelinek, N. Shauloff, R. Lebrón-Aguilar, J. Cernicharo, V. A. de la Peña O'Shea, H. A. Stone, P. L. de Andrés, G. Haller, G. J. Ellis, J. A. Martín-Gago, Nat. Commun. 12, 5937 (2021).
- *Tuning the Magnetic Anisotropy of Lanthanides on a Metal Substrate by Metal–Organic Coordination.* S. O. Parreiras, D. Moreno, B. Cirera, M. A. Valbuena, J. I. Urgel, M. Paradinas, M. Panighel, F. Ajejas, M. A. Niño, J. M. Gallego, M. Valvidares, P. Gargiani, W. Kuch, J. I. Martínez, A. Mugarza, J. Camarero, R. Miranda, P. Perna, D. Écija, Small 17, 2102753 (2021).
- *On-Surface Hydrogen-Induced Covalent Coupling of Polycyclic Aromatic Hydrocarbons via a Superhydrogenated Intermediate.* C. Sánchez-Sánchez, J. I. Martínez, N. Ruiz del Arbol, P. Ruffieux, R. Fasel, M. F. López, P. L. de Andres, J. A. Martín-Gago, J. Amer. Chem. Soc. 141, 3550-3557 (2019).
- *Highly Selective Covalent Organic Functionalization of Epitaxial Graphene.* R. Bueno, J. I. Martínez, R. Luccas, N. Ruiz del Árbol, C. Munuera, I. Palacio, F. J. Palomares, S. Thakur, J. M. Baranowski, W. Strupinski, M. F. López, F. Mompean, M. García-Hernández, J. A. Martín-Gago. Nat. Commun. 8, 15306 (2017).
- *Ultrafast Atomic Diffusion Inducing a Reversible $(2\sqrt{3}\times 2\sqrt{3})R30^\circ \leftrightarrow (\sqrt{3}\times\sqrt{3})R30^\circ$ Transition on Sn/Si(111):B.* W. Srour, D. G. Trabada, J. I. Martínez, F. Flores, J. Ortega, M. Abuín, Y. Fagot-Revurat, B. Kierren, P. Le Fèvre, A. Taleb-Ibrahim, D. Malterre, A. Tejeda, Phys. Rev. Lett. 114, 196101 (2015).
- *Fast Prediction of Adsorption Properties for Platinum Nanocatalysts with Generalized Coordination Numbers.* F. Calle-Vallejo, J. I. Martínez, J. M. García-Lastra, P. Sautet, D. Loffreda, Angew. Chem. Int. Ed. 53, 8316 (2014).

- *Graphene Etching on SiC Grains as a Path to Interstellar Polycyclic Aromatic Hydrocarbons Formation.* P. Merino, M. Svec, J. I. Martínez, P. Jelínek, P. Lacovig, M. Dalmiglio, S. Lizzit, P. Soukiassian, J. Cernicharo, J. A. Martín-Gago, Nat. Commun. 5, 3054 (2014).
- *Solvent-Induced Delamination of a Multifunctional Two Dimensional Coordination Polymer.* C. Hermosa, A. Gallego, O. Castillo, I. Berlanga, C. Gómez, E. Mateo, J. I. Martínez, F. Flores, A. Houlton, B. R. Horrocks, C. Gómez-Navarro, J. Gómez-Herrero, S. Delgado, F. Zamora, Adv. Mat. 25, 2141 (2013).
- *Tailored Formation of N-Doped Nanoarchitectures by Diffusion-controlled On-surface (Cyclo)-Dehydrogenation of Heteroaromatics.* A. L. Pinardi, G. Otero-Irureta, I. Palacio, J. I. Martínez, C. Sánchez-Sánchez, M. Tello, C. Rogero, A. Cossaro, A. Preobrajenski, B. Gómez-Lor, A. Jankaric, I. G. Stará, I. Stary, M. F. López, J. Méndez, J. A. Martín-Gago, ACSNano 7, 3676 (2013).
- *Improvement of STM Resolution with H-sensitized Tips.* J. I. Martínez, E. Abad, C. González, F. Flores, J. Ortega, Phys. Rev. Lett. 108, 246102 (2012).

C.2. Congress

The research results have been communicated in >70 national and international symposiums (35 oral, and 12 invited and keynote contributions). Latest (2018-2021): Riva2021 On-line, CMD2020GEFES, Graphene Week 2019 and 2018, 4th EMN Meeting on Computation and Theory (2018), Workshop on Synthetic Methods Across the Graphene Flagship (2018-2020), On-surface Synthesis (2018). Chair/organizer of international workshop EWEG/2D2018.

C.3. Research projects (2014-2021)

National Projects

- “Nueva generación de materiales multifuncionales para fotosíntesis artificial (FotoArt-CM)”. CAM. PI: Víctor de la Peña O’Shea. ICMM, IMDEA Energía, Nanociencia y Materiales, UAM, ICP. Period: 01/01/2019 – 31/12/2021. Ref.: S2018-NMT-4367. Funding: 1.083.374€.
- “Synthesis, characterization, and applications of nanomaterials: from Laboratory to Technology (nanoLabTech)”. MICINN. PI: Carlos Sánchez-Sánchez and José A. Martín-Gago (ICMM) Period: 01/09/2021 - 31/08/2024. Ref.: PID2020-113142RB-C21. Funding: 254.100€.
- “Síntesis Fotoquímica en Superficies (FotoSurf-CM)”. Comunidad de Madrid. PI: José A. Martín-Gago (ICMM), José Alemán (UAM) Period: 01/07/2021 - 30/06/2024. Ref.: Y2020/NMT-6469. Funding: 716.100€.
- “Materiales funcionales de baja dimensionalidad para (bio)sensores electroquímicos – FUNLDS”. MICINN. PI and C: José I. Martínez (ICMM) Period: 01/01/2018 – 30/09/2021. Ref.: MAT2017-85089-C2-1-R). Funding: 181.500€.

EU Projects

- “Gas and Dust: From the stars to the laboratory: Exploring the NANOCOSMOS”. European “Ideas” ERC Synergy Grants. PIs: José A. Martín-Gago, Christine Joblin, José Cernicharo. Period: 2014-2021. Ref.: ERC-2013-SYG-610256. Funding: 15.000.000 €.
- “Flagship Graphene: Future ICT, GrapheneCore1, GrapheneCore2, GrapheneCore3”, WP3. “Materials” Coordinator at ICMM: Mar García-Hernández. Periods: 2013-2016/2016-2018/2018-2020/2020-2023. Funding: 1.200.000 €/900.000€/650.000€/917.662,5€.

C.4. Contracts, technological or transfer merits (2016-2021)

Contracts - PI “Technological assistance contract” with the enterprise DYNASOL GESTION. “TRABAJOS DE SIMULACIÓN DE INTERACCIÓN DE OLIGÓMEROS DE BUTADIENO FUNCIONALIZADO SOBRE UNA SUPERFICIE DE SILICE”. Invoiced: 2000 € (2017)

- PI “Technological assistance contract” with the enterprise DYNASOL GESTION. “TRABAJOS DE SIMULACIÓN DE OLIGÓMEROS DE BUTADIENIL-LITIO ACOMPLEJADOS POR DIFERENTES COMPUESTOS QUÍMICOS”. Invoiced: 3000 € (2017)

Patents - R. Bueno, J. I. Martínez, R. Luccas, M. F. López, F. Mompeán, M. García-Hernández: “Procedimiento de obtención de un grafeno funcionalizado covalentemente con una molécula orgánica” (2016). National: P201630971 | European: EP17827054 (CSIC).