PROCEDIMIENTO DE SELECCIÓN DE PERSONAL INVESTIGADOR DOCTOR

CURRICULUM ABREVIADO (CVA) (Extensión máxima 4 páginas)

Part A. PERSONAL INFORMATION	**CVA date**	31/08/2021

First and Family name	Salvador Rodríguez Gómez (Balestra; SRG signed in papers)		
ID number	31738539B	Age	36
Researcher's identification numbers	Researcher ID	H-6283-2014	
	ORCID code	0000-0002-2163-2782	

A.1. Current position

Name of University / Institution	Spanish National Research Council (CSIC)			
Department	New Architectures in Materials Chemistry / Instituto de Ciencia de Materiales de Madrid (ICMM)			
Address and Country	Sor Juana Inés de la Cruz 3, 28049, Madrid, Spain			
Phone number	600320224	Email Address	s.rodriguez.gomez@csic.es	
Current position	Postdoctoral researcher		From	2020
Keywords	Physical chemistry of materials; Applied physics; Molecular simulation; Nanostructured materials; Sustainable Technology			

A.2. Education

Degree / Master / PhD	University / Country	Year
PhD. Biotecnología, *Ingeniería y Tecnología Química (RD99/2011)*	University Pablo de Olavide / Spain	2018
Msc. *Máster Interuniversitario de Ciencia y Tecnología de Coloides e Interfases*	University Pablo de Olavide / Spain	2012
Bsc. Physics, *Licenciado en Física*	University of Seville / Spain	2011

A.3. JCR articles, h-Index, thesis supervised

19 JCR papers (**17 Q1**, and 2 Q2), **9 JCR in first decile (D1)**: 7 in multidisciplinary Chemistry or Material Science (1 *J. Am. Chem. Soc.*, 1 *Angew. Chemie Int. Ed.*, 2 *Chem. Mater.*, 3 *J. Mater. Chem. A*), and 2 D1 in the specific areas of Inorganic and Nuclear Chemistry and Chemical Engineering (*Dalton Trans.*, and *ACS Sustain. Chem. Eng.*, resp.). **H-index = 13**. 293 total citations (Web of Science). 53.6 citations/year in the last 5 years. 115 citations in 2021 (until Sept.). One master thesis (MSc) supervised, and one Bachelor's Degree Final Project *(BSc)* supervised. One PhD thesis supervision in progress.

Part B. CV SUMMARY *(max. 3500 characters, including spaces)*

My research focuses on the development of methodologies for the realistic atomistic modelling of advanced materials. I study mainly nanoporous materials, particularly zeolites and metal-organic frameworks (MOFs), performing design, modelling, and structural and physicochemical characterization of materials, for energy, environmental and fine chemistry applications. **My main goal** is to achieve chemically-sound modelling at a realistic level to make reliable predictions and to better interpret experimental results. I have worked in multidisciplinary, theoretical and experimental environments, having collaborated with 66 co-authors from national and foreign institutions, in UK, France, Netherlands, and Korea. I have made 3 predoctoral and 1 postdoctoral visits to Universities of Amsterdam and Montpellier (accumulating one year), and one year postdoctoral visit in a world-class group in modelling nanoporous materials at the University of Montpellier-CNRS. Currently, I am a modelling researcher within an experimental world-class group in nanoporous materials synthesis, at the Instituto de Materiales de Madrid-CSIC (where I am in the second year as a Juan de la Cierva Formación fellow). **My main scientific achievements** include: **a)** the introduction and development of methodologies for modelling highly flexible zeolites and MOFs at unprecedented, crystallographic-like quality level, achieving a deep understanding of the role of cation and water dynamics on the structure and stability, **b)** designing materials for novel applications, *e.g.* controlled thermal expansion, by exploiting guest-induced structural deformation in MOFs, **c)** refined modelling for molecular adsorption- and separation-based technological applications in energy (hydrogen and hydrocarbon molecules), environmental sciences (capture of pollutant gases, such as CO_2 and CO), and fine chemistry (chiral

molecules separation, including drugs), and **d)** DFT-based potential development for accurate simulations of structural distortions in inorganic perovskites. I employ a combination of quantum (VASP, cp2k, CASTEP and Gaussian) and classical (LAMMPS, GROMACS, RASPA, and GULP) mechanics calculations, as well as enhanced sampling techniques (Metadynamics, using Plumed code), along with codes for structural design, analysis, and manipulation (SOD, ASE, etc.), achieving a direct comparison with experimental techniques, such as NMR, infrared, Raman, diffraction, molecular transport and sorption experiments. My own codes (FORTRAN, C, and Python) for data analysis and calculation are available, at github.com/salrodgom. My publication records are in Section A.3 and C.1 of the CVA, and the participation in conferences appears in section C.2. My **teaching activities** involve 234 grade-level hours of teaching at UPO and the supervision of a Bachelor's Degree Final Project, a master thesis, and an ongoing PhD thesis. I have participated in 13 project grants (2 international), and I have reviewed 16 scientific articles. Regarding **institutional responsibilities**, I am member of the Equality Commission of the ICMM-CSIC and in US I was a member of the Student Delegation and in *Junta de Facultad* of the Faculty of Physics.

Part C. RELEVANT ACCOMPLISHMENTS

C.1. Publications and contribution

19 JCR scientific papers (17 Q1 and 2 Q2), including 9 in first decile (D1) and 1 book chapter. For space reasons, I only explain in detail 6 D1 articles. In all the articles, I contributed to the development of the projects, calculations, discussion, and the writing of the papers. **(†)** indicates equal contributions as **first authors**. The number of citations is indicated in parenthesis (c: X) from WOS, and (x/y) indicates my author relative position.

1. Gao, ZR; **Balestra, SRG**; Li, J.; Camblor, MA. **(2/4) 2021**. HPM-16, a Stable Interrupted Zeolite with a Multidimensional Mixed Medium-Large Pore System Containing Supercages. *Angew. Chemie Int. Ed.,* 10.1002/anie.202106734. A new interrupted zeolite with extra-large pores was synthesised and characterised, with interest in gas mixture purification, energy storage and greenhouse gas capture applications. I predicted a complete and consistent set of hypothetical uninterrupted structures and conducted their structural modelling, which was necessary as input to accomplish the experimental structural characterization using advanced crystallographic synchrotron data. I was the only modelling researcher.
2. **Balestra, SRG (†)**; Vicent-Luna, JM **(†)**; Calero, S; Tao, S; Anta, JA. **(1/5) 2020**. Efficient modelling of ion structure and dynamics in inorganic metal halide perovskites. *J. Mater. Chem. A,* 8, 11824-11836, (c: 5) 10.1039/d0ta03200j. I developed interatomic potentials for modelling the important family of $PbCs(Br,I)_3$ energy materials. Firstly, I generated an *ab-initio* reference database of structures and energies, through DFT calculations, and then I wrote a genetic algorithm code to calculate the Buckingham cross-interactions coefficients that fit the database. I tested the results by modelling the materials stability, and further extension of this study to other temperatures was conducted by the co-authors.
3. Corella-Ochoa, MN; Tapia, JB; Rubin, HN; Lillo, V; González-Cobos, J; Núñez-Rico, JL; **Balestra, SRG**; Almora-Barrios, N; Lledós, M; Güell-Bara, A; Cabezas-Giménez, J; Escudero-Adán, EC; Vidal-Ferran, A; Calero, S; Reynolds, M; Martí-Gastaldo, C; Galán-Mascarós, JR. **(7/17) 2019**. Homochiral Metal-Organic Frameworks for Enantioselective Separations in Liquid Chromatography. *J. Am. Chem. Soc*., 141, 14306-14316, (c: 39) 10.1021/jacs.9b06500. A robust homochiral MOF was synthesised, which achieved for the first time high purity selective separation of enantiomeric drugs (>95%) in a molecular sieve. I first provided guidance on the capabilities of this material in enantiomer drug separation by conducting a systematic molecular simulation study (sorption and transport properties) which permitted the understanding of the experimental data. I did 90% of the modelling results.
4. Rigo, RT (†); **Balestra, SRG (†)**; Hamad, S; Bueno-Pérez, R; Ruiz-Salvador, AR; Calero, S; Camblor, MA. **(2/7) 2018**. The Si-Ge substitutional series in the chiral STW Zeolite Structure Type. *J. Mater. Chem. A*. 6, 15110-15122, (c: 14) 10.1039/c8ta03879a. The first experimental complete series of systematic replacement of Si by Ge atoms in a zeolite was performed, in the case of the STW zeolite. Also, for the first time, the heteroatom distribution in the whole compositional range of a zeolite was modelled. I worked with a co-author in this result, for which I wrote a code to determine an Effective Hamiltonian, used to study the stability of millions of configurations. We did the DFT structural optimization of the whole set of F-Ge environment configurations and computed their 19F NMR chemical shifts. I then modelled the theoretical NMR spectrum of F atoms, using the stability data computed with the Effective

Hamiltonian, and achieved a direct comparison with experiments. The good agreement allowed us to understand the features of the synthesis and structure, and assign unsolved F-NMR data to structural zeolite features that have been remained unknown for 25 years.

5. **Balestra, SRG**; Bueno-Pérez, R; Hamad, S; Dubbeldam, D; Ruiz-Salvador, AR; Calero, S. **(1/6) 2016**. Controlling Thermal Expansion: A Metal-Organic Frameworks Route. *Chem. Mater*. 28, 8296-8304, (c: 26) 10.1021/acs.chemmater.6b03457. A conceptual design is introduced for the first time, to use MOFs as potential materials for the elaboration of mechanical barriers to control thermal expansion, which is useful for applications in systems exposed to abrupt temperature changes, such as in aerospace or microelectronics. A computational study is carried out, allowing the analysis of the effect of temperature and the nature of the molecules encapsulated in the pores on the thermal expansion of the system. We performed a comprehensive analysis of host-guest interactions. I had the original idea behind the project and I performed all the calculations.
6. **Balestra, SRG;** Hamad, S; Ruiz-Salvador, A. Rabdel; Domínguez-García, V; Merkling, PJ; Dubbeldam, D; Calero, S. **(1/7) 2015**. Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. *Chem. Mater*. 27, 5657-5667, (c: 27) 10.1021/acs.chemmater.5b02103. A theoretical description of the structural features of highly flexible nanoporous materials at quality comparable to crystallographic experiments was missing, despite the rise of theoretical methods in the last three decades. For that reason, in this article we developed a novel methodology, combining Monte Carlo simulations, Energy Minimisation and Molecular Dynamics. We modelled the structural changes in RHO zeolite with different compensating cations and various temperatures and degrees of hydration. The opening of the zeolite pore windows was found to correlate with either the cation polarising power, and the degree of humidity. I wrote the program that called two external codes to conduct the calculations, as well the code used for the analysis of the pore windows flexibility. The work opened a path to the theoretical study of molecular valves, with applications to gas purification, sensing and energy storage. I performed all the calculations.
7. Gónzalez-Galán, C; **Balestra, SRG (*,CA)** *et al.* **(2/6) 2021**. *Dalton Trans.,* 50, 1808-1815
8. Pérez-Carbajo *et al.*, **(2/4) 2020**, *Microp. Mesop. Mater.* 293, 109808-1-109808-6 (c: 3)
9. López-Salas *et al*., (7/13) **2019**, *ACS Sustain. Chem. & Eng.* 7, 17565-17573 (c: 29)
10. Pérez-Carbajo *et al.*, **(3/9) 2018**, *ACS Applied Materials & Interfaces,* 10, 20512-20520 (c:13)
11. Bueno-Pérez *et al.*, **(2/7) 2018**, *Chemistry: A European Journal*, 24, 4121-4132 (c: 7)
12. J Min *et al.*, **(4/8) 2018**, *Langmuir,* 34, 4774-4779 (c: 8)
13. Sánchez-Laínez *et al.,* **(4/9) 2017**, *Journal of Materials Chemistry A*. 5, 25601-25608 (c: 28)
14. Gutiérrez-Sevillano *et al.,* **(8/9) 2016**. *Chemistry: A European Journal,* 22 (c: 13)
15. Slawek *et al.,* **(4/6) 2016**, *J. Physical Chemistry C*. 120-44, 25338-25350 (c:14)
16. Gómez-Álvarez *et al.* **(3/4) 2016,** *J. Physical Chemistry C*. 120, 23254-23261 (c: 15)
17. Torres-Knoop *et al*. **(2/5) 2015**, *ChemPhysChem*. 16, 532-535 (c: 13)
18. Hamad *et al.*, **(2/5) 2014**, *Journal of Solid-State Chemistry (c: 28)*
19. **Balestra, SRG** *et al*., **(1/5) 2013**, *J. Physical Chemistry C*. 117, 11592-11599 (c: 14)

C.2. Conferences and meetings

I have presented 4 oral and 5 poster contributions in international/European congresses and meetings. I have also participated in other 6 oral and 13 poster contributions. The complete list of contributions is available in my online CVN: cvn.fecyt.es/editor/cvnOnline/0000-0002-2163-2782. Below, I list the data concerning the presented 4 oral contributions.

1. Balestra, SRG; *et al.,* Controlling Thermal Expansion: A metal–Organic Frameworks Route. *Workshop of Molecular Simulation of Nanoporous Materials and Ionic Liquids*, 2016, Delft
2. Balestra, SRG; *et al.,* Computational Study of ethanol/butanol/pentanol/water separation in hierarchical pure silica zeolites, *40ª Reunión Ibérica de Adsorción*, 2016, Évora, Portugal
3. Balestra, SRG; *et al*. Distortion mechanisms in RHO zeolites: Effects of the cation type and the loading of CO_2, *10th Internat. Symp. Characteriz. Porous Solids*, 2014, Granada, Spain
4. Balestra, SRG; *et al.,* Simulation study of structural phase transition of RHO zeolite, *Eur. Congress and Exhibition on Adv. Mater. and Proc.* (EUROMAT), 2013, Seville, Spain

C.3. R&D and innovation projects, grants, and contracts

I have participated in 2 international, 4 national, and 1 regional (Andalusia) projects, 2 competitive granted-contracts, 3 non-competitive contracts, and 3 competitive mobility

grants. The complete list is available in cvn.fecyt.es/editor/cvnOnline/0000-0002-2163-2782. The more relevant items are listed below:

1. Granted contract. FJC2018-035697-I. *Ayudas para contratos* **Juan de la Cierva-Formación** 2019. *Agencia Estatal de Investigación, Ministerio de Ciencia e Innovación (AEI-MCIn).* 2020-2022. 50,000 EUR. Competitive grant. Principal investigator (**PI**)
2. Contract. H-2020 Action, KAUST-II. 2019. *Centre National de la Recherche Scientifique* (CNRS), Montpellier, France, 2019-2020. Postdoctoral researcher and team member.
3. Granted contract. BES-2014-067825. ***Ayudas para Contratos Predoctorales para la Formación de Doctores (FPI)*** 2014. *Ministerio de Economía y Hacienda* (MINECO), 2015-2019. 88,400 EUR. Competitive grant. **PI**
4. Mobility Grants. EEBB-I-18-13045, EEBB-I-2017-12125, and EEBB-I-2016-11628. *Estancias Breves FPI* 2017, 2016, and 2015. MINECO, 2 Montpellier (France) and 1 in Amsterdam (Netherlands), 2018, 2017, 2016 (5,130; 4,930, and 2,951 EUR, resp.). **PI**
5. Project. ERC-279520. Towards more efficient materials for technological applications. *EU 7th Framework Program (FP7/2007-2013) under grant agreement nº 262336*. Calero, S (University Pablo de Olavide). 2012-2016. Contracted researcher and team member.

C.4. Outreach activities and results exploitation

1. Open access published software. GAIAST program (Genetic Algorithm Ideal Adsorption Theory, DOI:10.5281/zenodo.596674), FLAMA code (Genetic Algorithm to fit Potentials, DOI:10.5281/zenodo.5361088), White Rabbit (Analysis of crystalline structures, cavities, and windows, DOI:10.5281/zenodo.5361665) and 12 others, available in github.com/salrodgom.
2. Dissemination of science to society. 2 articles in *MoleQla* (ISSN-e 2173-0903) in 2012 (titles: "Diagrama de fases de un sistema de esferas duras" y "El Método de Monte Carlo").
3. I have contributed in science outreach events, such as the ***Feria de la Ciencia*** and ***Science Talks*** in pubs.

C.5. Stays and Internationalization

Almost two years of research experience abroad (see below). I have generated a network of 25 foreign co-authors with whom I keep active collaborations.

1. Two short-stays in the University of Amsterdam (UvA), Amsterdam, Netherlands, in 2014 and 2016 (91 days and 60 days, respectively) (PI: David Dubbeldam)
2. Two short-stays in the University of Montpellier, Institut Charles Gerhardt, Montpellier, France in 2017 and 2018 (114 and 63 days, respectively) (PI: Guillaume Maurin)
3. A long-stay in the University of Montpellier-CNRS, France, as postdoctoral contract (365 days) (PI: Rocío Semino).

C.6. Teacher or researcher recognition or accreditation

1. ANECA Teacher Accreditations. **Profesor Ayudante Doctor**, **Profesor Contratado Doctor** y **Profesor Universidad Privada** (2018)
2. Researcher Recognitions, Mentions or Awards**: Seal of Excellence** Award of the European Research Commission 2019, ***Mención Doctorado Internacional*** and ***Premio Extraordinario Doctorado*** 2019.

C.7. Official Education

1. Teaching: 234 hours of lecturer in the Pablo de Olavide University (2016-2019)
2. Supervision of MSc thesis. **Student**: Francisca Aguilar Lineros, **Title**: Enrejados zeolíticos de Imidazol (ZIF) con ligandos mixtos para el estudio de la expansión térmica en materiales porosos, **Master**: Máster Oficial de Simulación Molecular, **Institution**: Universidad Internacional de Andalucía, **Year**: 2018-2019.
3. Supervision of First Degree thesis. **Student**: José Manuel González Montiel, **Title**: Effect of Structural Flexibility on the Adsorption and Diffusion of CH_4 and CO_2 in ITQ-29 and ITQ-50 zeolites, **Degree**: Environmental Science, **Institution**: Pablo de Olavide University, 2015.

C.8. Reviewing activities

External reviewer for several journals, including first quartiles in my field, with 16 verified reviews in the last 5 years: 1 *J. Chem. Phys.* (AIP), 1 *Microp. Mesop. Materials* (Elsevier), 2 *J. Nanostructure Chem.* (Springer Nature), 6 *Adsorption* (Springer Nature), 4 *AICHE Journal* (Wiley), 1 *Zeit. Kristallog. – Cryst. Mater.* (De Gruyter), and 1 *Geoscience* (MDPI).