Salvador Rodríguez–Gómez (Balestra)

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salrodgom.github.io

Bio

I was born in Cádiz (Spain) in 1985. I graduated in Physics in 2011 in the University of Seville (US). I attended the University of Granada (UGR) during the course 2008/09, with the SENECA Visit Program, to specialise in Complex Systems, Computing and Statistical Mechanics. I did the "Master of Science and Technology of Colloids and Interfaces" at the University Pablo de Olavide, in Seville, (UPO) focusing on Molecular Physics studies and Simulation Techniques. From 2012 to 2017 I worked as a technician supporting the research in a Starting-Grant European Project on computer studies in nanoporous materials. My role consisted in developing simulation techniques and programming to support the project. During these years I participated in several research projects, detailed in the CV. In 2015 I got a research grant: a predoctoral contract for the training of PhDs, of competitive nature, focused on the study of the separation of organic isomers by porous materials. During this phase I participated in works that lead to scientific publications in high impact journals, such as *Chemistry of Materials*, or *Journal of Material Chemistry A* and I also made contributions in international conferences. In 2018 I defended my doctoral thesis with an outstanding **cum laude** qualification (Atomistic insights into flexibility of nanoporous crystals). Subsequently, I obtained a postdoctoral contract under the one-year postdoctoral guidance period. In 2018, I have published four articles in high impact journals, and I have started collaborations with several groups at a national and international level to expand my research to new horizons. I also continue working with the collaborators that I had during the thesis. In these years I have made four predoctoral short-stays, two in Amsterdam (Netherlands), and two in Montpellier (France). The summary of my research is how the phase transitions in nanoporous (flexible) crystals influence the adsorption and transport of molecules (and vice versa).

Keywords Molecular Simulation, Complex Systems, DFT, Nonequilibrium Statistical Physics, and Criticality

Education

- **Pablo de Olavide University, UPO** — **Seville, Andalusia, Spain**
  PhD Student in the Physical–Chemistry Division — *2012 – 2018*
  - Thesis: Atomistic insights into flexibility of nanoporous crystals, (ISBN: 978-84-09-00004-3)
  - Advisors: Prof. Sofía Calero–Díaz (UPO) and Dr. David Dubbeldam (UvA)

  Master Degree in Science and Technology of Colloids and Interfaces — *2011 – 2012*
  - Thesis: *Estudio de la transición de fase estructural de la zeolita RHO mediante simulación*
  - Advisor: Prof. Sofía Calero–Díaz
- **University of Seville, US** — **Seville**
  Bachelor & Master Degree in Physics, Faculty of Physics — *2004 – 2011*
  Visit program grant *SICUE/SENECA* from *Programa de Ayudas para la Movilidad de Estudiantes* in the **University of Granada, UGR** — *2008 – 2009*

Experience

- **Pablo de Olavide University** — **Seville**
  Postdoc position and PhD. Student Researcher — *2015 – 2019*
  - Researcher of National Plan R & D & i, through a competitive fellowship: "Ayuda para contratos predoctorales para la formación de doctores"

Project: *Identificación y diseño de estructuras porosas para procesos de separación*
* *de isómeros orgánicos*, CTQ2013-48396-P.
Principal Investigator (PI): Prof. Sofía Calero–Díaz *2015 – 2019*

Project: *Control ad hoc de la flexibilidad de estructuras porosas para su uso en captura y*
* *liberación de fluidos*, CTQ2016-80206-P.
Principal Investigator (PI): Prof. Sofía Calero–Díaz *2017 – 2019*

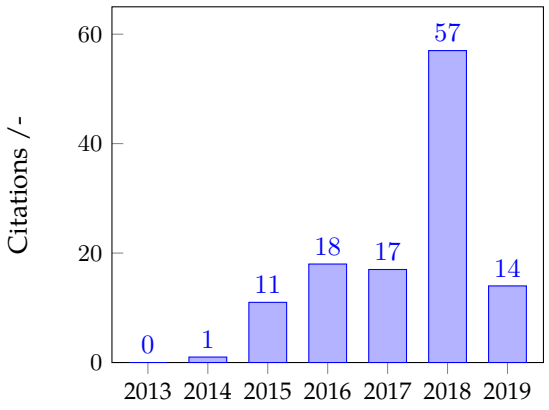
- **Pablo de Olavide University** **Seville**
  Technician supporting the research *2012 – 2015*
  - Researcher of ERC Starting Grant
    * Project: Towards more efficient materials for technological processes.
      EU 7th Framework Program, code: 279520, PI: Prof. Sofía Calero–Díaz *2012–2015*
  - Researcher of Andalusian Plan R & D & i
    * Project: Physical–Chemistry of interfaces and condensed phases [FQM-319].
      PI: Dr. Patrick Merkling *2012 – present day*
    * Project: *Captura, Almacenamiento y Fotoconversión de CO_2*
      procedente de Emisiones Industriales Motriz. P12-FQM-1851
      PI: Prof. Sofía Calero–Díaz *2014 – now*
  - Researcher of National Plan R & D & i
    * Project: Molecular Simulation in porous crystalline materials as tools to optimize
      processes of technological and environmental interest. CTQ2010-16077
      PI: Prof. Sofía Calero–Díaz *2011 – 2013*

- **University of Seville** **Seville**
  Contributor Student

  Natural Computation Group in the Mathematical Analysis Division
  – Project: Cellular Automatas and Mathematica–Physics
  PI: Dr. Juan Carlos García–Vázquez *2010 – 2012*

Scientific Contributions:
ResearcherID: H-6283-2014
ORCID ID: 0000-0002-2163-2782

I have published 13 scientific articles in journals indexed in Web of Science (WOS), of which eleven are Q_1 and two are Q_2 in at least one of the following three categories: *Materials Science, Multidisciplinary* and *Physical Chemistry*. It should be noted that five of these articles appear in the **First Decil** journals (D_1) in both categories: two papers published in *Journal of Materials Chemistry A* (JIF: 9.931, RSC), two papers in *Chemistry of Materials* (IF: 9.466 , ACS) and another D1 in the category *Materials Science, Multidisciplinary*, published in *ACS Applied Materials & Interfaces* (JIF: 8.097, ACS).
WOS reports 86 citations, with a notable increase in 2018 (with 43 cites), a trend also reported by Scholar Google, with 118 total citations, 68 of which since 2018. The H index associated with these articles and citations is 6 in WOS and 7 in Scholar Google.



- **Articles in peer-reviewed journals** 13 peer-reviewed journal papers, total times cited: 118
  Data from `Scholar Google` and Web of Science

1. Reus T. Rigo, Salvador R. G. Balestra, Said Hamad, Rocio Bueno-Perez, A. Rabdel Ruiz-Salvador, Sofía Calero, and Miguel A. Camblor. The Si–Ge substitutional series in the chiral STW zeolite structure type. *Journal of Materials Chemistry A*, 6(31):15110–15122, 2018. `DOI:10.1039/c8ta03879a`

2. Julio Perez-Carbajo, Ismael Matito-Martos, Salvador R. G. Balestra, Mihalis N. Tsampas, Mauritius C. M. van de Sanden, José A. Delgado, V. Ismael Águeda, Patrick J. Merkling, and Sofia Calero. Zeolites for CO_2–CO–O_2 separation to obtain CO_2-neutral fuels. *ACS Applied Materials & Interfaces*, 10(24):20512–20520, may 2018. DOI:10.1021/acsami.8b04507
3. Jung Gi Min, Azahara Luna-Triguero, Youngchul Byun, Salvador R. G. Balestra, Jose Manuel Vicent-Luna, Sofia Calero, Suk Bong Hong, and Miguel A. Camblor. Stepped propane adsorption in pure-silica ITW zeolite. *Langmuir*, 34(16):4774–4779, apr 2018. DOI:10.1021/acs.langmuir.8b00628
4. Rocio Bueno-Perez, Salvador R. G. Balestra, Miguel A. Camblor, Jung Gi Min, Suk Bong Hong, Patrick J. Merkling, and Sofia Calero. Influence of flexibility on the separation of chiral isomers in STW-type zeolite. *Chemistry - A European Journal*, 24(16):4121–4132, feb 2018. DOI:10.1002/chem.201705627
5. Javier Sánchez-Laínez, Adrián Veiga, Beatriz Zornoza, Salvador R. G. Balestra, Said Hamad, A. Rabdel Ruiz-Salvador, Sofia Calero, Carlos Téllez, and Joaquín Coronas. Tuning the separation properties of zeolitic imidazolate framework core–shell structures via post-synthetic modification. *Journal of Materials Chemistry A*, 5(48):25601–25608, 2017. DOI:10.1039/c7ta08778k
6. Salvador R.G. Balestra, Rocío Bueno-Pérez, Said Hamad, David Dubbeldam, A Rabdel Ruiz-Salvador, and Sofia Calero. Controlling Thermal Expansion: A metal–Organic Frameworks Route. *Chemistry of Materials*, 2016. DOI:10.1021/acs.chemmater.6b03457
7. Juan José Gutiérrez-Sevillano, Sofía Calero, Said Hamad, Ricardo Grau-Crespo, Fernando Rey, Susana Valencia, Miguel Palomino, Salvador R. G. Balestra, and A. Rabdel Ruiz-Salvador. Critical role of dynamic flexibility in ge-containing zeolites: Impact on diffusion. *Chemistry - A European Journal*, 22(29):10036–10043, jun 2016. DOI:10.1002/chem.201600983
8. Paula Gómez-Álvarez, Julio Perez-Carbajo, Salvador RG Balestra, and Sofia Calero. Impact of the nature of exchangeable cations on LTA-type zeolite hydration. *The Journal of Physical Chemistry C*, 120(40):23254–23261, 2016. DOI:10.1021/acs.jpcc.6b06916
9. Andrzej Sławek, José Manuel Vicent-Luna, Bartosz Marszałek, Salvador Rodríguez-Gómez Balestra, Wacław Makowski, and Sofia Calero. Adsorption of n-alkanes in MFI and MEL: Quasi-equilibrated thermodesorption combined with molecular simulations. *The Journal of Physical Chemistry C*, 2016. DOI:10.1021/acs.jpcc.6b06957
10. Salvador R.G. Balestra, Said Hamad, A. Rabdel Ruiz-Salvador, Virginia Domínguez-García, Patrick J. Merkling, David Dubbeldam, and Sofía Calero. Understanding nanopore window distortions in the reversible molecular valve zeolite RHO. *Chemistry of Materials*, 27(16):5657–5667, 2015. DOI:10.1021/acs.chemmater.5b02103
11. A. Torres-Knoop, Salvador R. G. Balestra, R. Krishna, S. Calero, and D. Dubbeldam. Entropic separations of mixtures of aromatics by selective face-to-face molecular stacking in one-dimensional channels of metal–organic frameworks and zeolites. *ChemPhysChem*, 16(3):532–535, 2015. DOI:10.1002/cphc.201402819
12. Said Hamad, Salvador R.G. Balestra, Rocio Bueno-Perez, Sofia Calero, and A. Rabdel Ruiz-Salvador. Atomic charges for modeling metal–organic frameworks: Why and how. *Journal of Solid State Chemistry*, 223:144 – 151, 2015. DOI:10.1016/j.jssc.2014.08.004 . Metal-organic Frameworks-Promising Solid State Porous Materials in 21st Century
13. Salvador R.G. Balestra, Juan José Gutierrez-Sevillano, Patrick J. Merkling, David Dubbeldam, and Sofía Calero. Simulation study of structural changes in zeolite RHO. *Journal of Physical Chemistry C*, 117(22):11592–11599, 2013. DOI:10.1021/jp4026283

- **Book Chapter**

1. Juan Carlos García-Vázquez, Salvador Rodríguez-Gómez, and Fernando Sancho-Caparrini. Biham–Middleton–Levine Traffic Model in two–dimensional hexagonal lattice. Springer Proceedings in Complexity, pages 943–948. Springer International Publishing, 2013. DOI:10.1007/978-3-319-00395-5_113

- **Popular science articles (Spanish)**

1. Salvador Rodríguez-Gómez. El método Monte Carlo. *MoleQla*, 5:133 – 135, 2012. ISSN 2173-0903
2. Salvador Rodríguez-Gómez. Diagrama de fases de un sistema de esferas duras. *MoleQla*, 6:161–162, 2012. ISSN 2173-0903

All my scientific works have been presented both in national and international conferences, being previously evaluated by admission committees. I have participated in international conferences, such as the triennial *International Conference on Zeolites* (Rio de Janeiro, 2016), the most outstanding in the area of porous materials, and in others like the *10th International Symposium on the Characterization of Porous Solids*, COPS), and *6th Internaltion FEZA Conference*, also of global in nature, which are relevant in the branches of adsorption and separation of porous materials. I have also presented papers in 12 other conferences of European and Ibero-American nature. I have made four oral presentations in international conferences.

- **Oral contributions in congress**

1. Salvador R.G. Balestra, Rocío Bueno-Pérez, Said Hamad, David Dubbeldam, A Rabdel Ruiz-Salvador, and Sofia Calero. Controlling Thermal Expansion: A metal–Organic Frameworks Route. In *1st Workshop of Molecular Simulation of Nanoporous Materials and Ionic Liquids*, Seville–Delft, 2016
2. Salvador R. G. Balestra, Jose Manuel Ortiz-Roldán, Rocío Bueno-Pérez, Said Hamad, A. Rabdel Ruiz-Salvador, and Sofía Calero. Computational study on ethanol/butanol/pentanol/water separation in hierarchical pure silica zeolites. In *40th Reunión Ibérica de Adsorción (RIA)*, Septembre 2016. Évora, Portugal
3. J. M. Ortiz-Roldán, A. R. Ruiz-Salvador, S. Calero, S. R. G. Balestra, C. Richard A. Catlow, E. García-Pérez, F. Montero-Chacón, and S. Hamad. Ordered microporous metals. In *EuCheMS Chemistry Congress*, 2016. Seville
4. A. Sławek, J. M. Vicent-Luna, S. R.G. Balestra, W. Makowski, and S. Calero. Molecular simulations of adsorption of n-alkanes on high silica ZSM-5 zeolite applied in the quasi-equilibrated thermodesorption. In *The 7th International Conference on Silicate Materials: BaltSilica*, Kaunas, Lithuania, may 2016
5. J.E. Pérez-Izquierdo, S.R.G. Balestra, S. Calero, and P. Gómez-Álvarez. Effect of Si/Al ratio on water hydration in LTA-type zeolites. In *40th Reunión Ibérica de Adsorción (RIA)*, Évora, Portugal, sep 2016
6. A. R. Ruiz-Salvador, S. R. G. Balestra, R. Bueno-Pérez, S. Hamad, and S. Calero. Modeling nanoporous solids with force fields based approaches. In *1st International Workshop on Software Solutions for ICME*, Kerkrade, Países Bajos, 2014
7. Salvador R. G Balestra, S. Hamad, A. Rabdel Ruiz-Salvador, P. J. Merkling, and S. Calero. Distortion mechanisms in RHO zeolites: Effects of the cation type and the loading of carbon dioxide. In *10th International Symposium on the Characterization of Porous Solids (COPS-X)*, Granada, 2014
8. Salvador R. G Balestra, J. J. Gutiérrez-Sevillano, P. J. Merkling, D. Dubbeldam, and S. Calero. Simulation study of structural phase transition of RHO zeolite. In *European Congress and Exhibition on Advanced Materials and Processes (EUROMAT2013)*, Seville, 2013
9. J. C. García-Vázquez, F. Sancho-Caparrini, and S. Rodríguez-Gómez. Biham-Middleton-Levine Traffic Model in Two Dimensional Hexagonal Lattice. In *European Conference on Complex Systems*, Bruseles, 2012

- **Poster contributions in congress**

1. A. Luna–Triguero, J. M. Vicent-Luna, S. R. G. Balestra, and S. Calero. Guest induced flexibility of metal-organic frameworks for butadiene capture. In *41a Reunión Ibérica de Adsorción, 3o Simposio Iberoamericano de Adsorción*, Gijón, Principality of Asturias, Spain, sep 2018
2. I. Matito–Martos, J. M. Vicent-Luna, S. R. G. Balestra, and S. Calero. High ammonia uptake in azolate metal - organic framework with open metal sites. In *41a Reunión Ibérica de Adsorción, 3o Simposio Iberoamericano de Adsorción*, Gijón, Principality of Asturias, Spain, sep 2018
3. J. M. Ortiz-Roldán, A. R. Ruiz-Salvador, S. Calero, S. R. G. Balestra, C. Richard A. Catlow, E. García-Pérez, F. Montero-Chacón, and S. Hamad. Ordered microporous metals. In *EuCheMS Chemistry Congress*, 2016. Seville
4. S. R. G. Balestra, R. Bueno-Perez, S. Hamad, Á. R. Ruíz-Salvador, and S. Calero. Controlling thermal expansion using metal-organic frameworks: A new perspective. In *6th EuCheMS Chemistry Congresss*, Sevilla, Andalusia, Spain, sep 2016
5. R. Bueno–Perez, S. R. G. Balestra, P. Merkling, and S. Calero. Effect of flexibility on structural and chiral separation performance of zeolites. In *6th EuCheMS Chemistry Congresss*, Sevilla, Andalusia, Spain, sep 2016

6. J. E. Pérez–Carbajo, I. Matitos-Martos, S. R. G. Balestra, M.C.M. van de Sanden, and S. Calero. Zeolites for $CO_2/CO/O_2$ separation to obtain CO_2 -neutral fuels. In *6th EuCheMS Chemistry Congresss*, Sevilla, Andalusia, Spain, sep 2016
7. R. Bueno-Pérez, S.R.G. Balestra, S. Calero, and P.J. Merkling. Computational infrared spectra of zeolites as a characterization tool. In *40th RIA*, Évora, Portugal, sep 2016
8. José Manuel Ortiz Roldán, Ángel Rabdel Ruíz Salvador, Salvador Rodríguez Gómez, Sofía Calero Díaz, Elena García Pérez, Francisco Montero Chacón, Richard Catlow, and Said Hamad Gómez. Theoretical study of the stability of template-grown ordered metal nanofoams. In *40a Reunión Ibérica de Adsorción (RIA)*, 2016. Évora, Alentejo, Portugal
9. S.R.G. Balestra, J.M. Ortiz Roldán, S. Hamad, A. R. Ruiz-Salvador, and S. Calero. Hierarchical Na,Ca-zeolites for biofuel/water separation: A simulation study. In *18th International Zeolite Conference*, Jun 2016. Rio de Janeiro, Brasil
10. R. Bueno-Pérez, S.R.G. Balestra, P.J. Merkling, and S. Calero. Effect of the flexibility in the enantiomeric selectivity of STW zeolite. In *18th International Zeolite Conference*, Rio de Janeiro, Brasil, june 2016
11. J.E. Pérez-Izquierdo, S.R.G. Balestra, R. Bueno-Pérez, and S. Calero. Exploiting germanosilicate flexibility for alkane isomers separation. Rio de Janeiro, Brasil, june 2016
12. S.R.G. Balestra, A.R. Ruiz-Salvador, and S. Calero. About the possibility of control the thermal expansion using metal organic frameworks. In *1er Simposio sobre Propiedades y Aplicaciones de MOFs y COFs*, abril 2015. Granada, España
13. A. R. Ruiz-Salvador, S. Hamad, S. R. G. Balestra, A. Gomez, D. W. Lewis, and S. Calero. Flexibility of isotypic topologies: zeolites vs ZIFs ilustrated by GIS and LTA frameworks. In *6th International Federation of European Zeolite Associations Conference (FEZA)*, Septiembre 2014. Leipzig, Alemania
14. J. J. Gutiérrez-Sevillano, S. Calero, S. Hamad, S. R. G. Balestra, R. Grau-Crespo, F. Reya, S. Valencia, and A. R. Ruiz-Salvador. Anomalous breathing behaviour in Ge-LTA zeolite and its implication in enhanced diffusion. In *10th International Symposium on the Characterization of Porous Solids (COPS)*, Mayo 2014. Granada, España
15. Rodríguez-Gómez, S., J. J. Gutiérrez-Sevillano, G. Sánchez-Crespo, and S. Calero. Estudio del efecto de la temperatura, presión y tipo de catión sobre la estructura flexible de la zeolita RHO mediante técnicas de simulación molecular. In *XVIII Congreso de Física Estadística (FISES)*, Octubre 2012. Mallorca, España
16. Rodríguez-Gómez, S., J. J. Gutiérrez-Sevillano, G. Sánchez-Crespo, and S. Calero. Simulation study of structural transitions of rho zeolite during adsorption of carbon dioxide. In *XXXVII Reunión Ibérica de Adsorción (RIA)*, 2012. Sevilla, España
17. Gutiérrez-Sevillano, J. J., S. Calero, C. Ania, J. B. Parra, J. Kapteijn, F.and Gascón, S. R. G. Balestra, and S. Hamad. Towards a transferable set of charges to model zeolitic imidazolate frameworks: A combined experimental-theoretical resaearch. In *XXXVII Reunión Ibérica de Adsorción (RIA)*, 2012. Sevilla, España
18. Gutiérrez-Sevillano, J. J., F. Siperstein, S. R. G. Balestra, and S. Calero. On the performance of ETS-10 for CO_2/CH_4 and CO_2/N_2 separations. In *XXXVII Reunión Ibérica de Adsorción (RIA)*, 2012. Seville, España

- **Software**

  – Salvador R.G Balestra, Rocio Bueno-Perez, and Sofia Calero. GAIAST: A Genetic Algorithm for the Ideal Adsorbed Solution Theory. *Zenodo*, nov 2016. `DOI:10.5281/zenodo.165844`

- **Peer-reviews**
  I have reviwed several works in two journals: *Zeitschrift für Kristallographie - Crystalline Materials* (De Gruyter) and *Adsorption* (Springer).

Short-stays

I have made four short-stays (a total of 10 months and 22 days) in the last four years, in the universities of Amsterdam and Montpellier II. The visits have been hosted by leading researchers of global reference in molecular simulation and porous materials science; Dr. David Dubbeldam and Prof. Dr. Guillaume Maurin, respectively. These short-stays have generated various publications and there is ongoing work, in the process of reviewing.

- **University of Amsterdam** **Amsterdam, Netherlands**
  Van't Hoff Institute for Molecular Sciences *May/2014–July/2014*
- **University of Amsterdam** **Amsterdam, Netherlands**
  Van't Hoff Institute for Molecular Sciences
  Ayudas para contratos predoctorales para la formación de doctores 2015 *May/2016–June/2016*
- **University of Montpellier II** **Montpellier, France**
  Institut Charles Gerhardt, (*Dynamique et Adsorption dans les Matériaux Poreux*)
  Ayudas para contratos predoctorales para la formación de doctores 2016 *March/2017–July/2017*
- **University of Montpellier II** **Montpellier, France**
  Institut Charles Gerhardt, (*Dynamique et Adsorption dans les Matériaux Poreux*)
  Ayudas para contratos predoctorales para la formación de doctores 2017 *May/2018–June/2018*

Educational Activities

- **Teaching in classroom, 232 hours**
  Pablo de Olavide University **Seville**
  Chemical Termodynamics and Kinetics, tutorials. Biotechnology Bachelor's Degree *93 hours/2015-2018*
  Environmental Pollution, tutorials. Environmental Sciences Bachelor's Degree *105 hours/2016-2019*
  Chemistry, lectures. Environmental Sciences Bachelor's Degree *16 hours/2019*
  Pharmaceutical industry and drug design, lectures. Biotechnology Bachelor's Degree *9 hours/2019*
  Organic Chemistry, lectures. Environmental Sciences Bachelor's Degree *9 hours/2019*
- **Supervising End of Course Projects**
  Pablo de Olavide University **Seville**
  Title: Effect of structural flexibility on the adsorption and diffusion of CH_4 and CO_2 in ITQ-29 and ITQ-50 zeolites, Obtained qualification: 9.8/10.0
  Co-supervisor: Prof. Sofía Calero Díaz,
  Student: José Manuel González Montiel *April/2015*
- **Supervising PhD Canditate**
  Pablo de Olavide University **Seville**
  Title: Diffusion Patterns in nanoporous materials containing defects
  Co-supervisor: Prof. Sofía Calero Díaz,
  Candidate: María Pilar Leal Fernández *2018–now*

Core Technical Skills

Computer Programming Profit Level: Fortran (95/2003), shell scripting, and LaTeX. Basic Level: C/C++, Python, and parallel tools like OpenMPI and CUDA
Molecular Simulation Software RASPA, GULP, VASP, CP2K, LAMMPS and DL_POLY
Visulization The Visualization Toolkit (VTK), VMD
OS GNU/Linux and Windows

Updated: 3rd March 2019

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[1] Salvador R.G. Balestra, Juan José Gutierrez-Sevillano, Patrick J. Merkling, David Dubbeldam, and Sofía Calero. Simulation study of structural changes in zeolite RHO. *Journal of Physical Chemistry C*, 117(22):11592–11599, 2013. DOI:10.1021/jp4026283 .

[2] Salvador R.G. Balestra, Said Hamad, A. Rabdel Ruiz-Salvador, Virginia Domínguez-García, Patrick J. Merkling, David Dubbeldam, and Sofía Calero. Understanding nanopore window distortions in the reversible molecular valve zeolite RHO. *Chemistry of Materials*, 27(16):5657–5667, 2015. DOI:10.1021/acs.chemmater.5b02103 .

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[4] Salvador R.G. Balestra, Rocío Bueno-Pérez, Said Hamad, David Dubbeldam, A Rabdel Ruiz-Salvador, and Sofia Calero. Controlling Thermal Expansion: A metal–Organic Frameworks Route. *Chemistry of Materials*, 2016. DOI:10.1021/acs.chemmater.6b03457 .

[5] Rocio Bueno-Perez, Salvador R. G. Balestra, Miguel A. Camblor, Jung Gi Min, Suk Bong Hong, Patrick J. Merkling, and Sofia Calero. Influence of flexibility on the separation of chiral isomers in STW-type zeolite. *Chemistry - A European Journal*, 24(16):4121–4132, feb 2018. DOI:10.1002/chem.201705627 .

[6] J.J. García-Vázquez, S. R. G. Balestra, and F. Sancho-Caparrini. Non-trivial collective behavior in low dimensional cellular automata. Unpublished, 2013.

[7] Juan Carlos García-Vázquez, Salvador Rodríguez-Gómez, and Fernando Sancho-Caparrini. Biham–Middleton–Levine Traffic Model in two–dimensional hexagonal lattice. Springer Proceedings in Complexity, pages 943–948. Springer International Publishing, 2013. DOI:10.1007/978-3-319-00395-5_113 .

[8] Paula Gómez-Álvarez, Julio Perez-Carbajo, Salvador RG Balestra, and Sofia Calero. Impact of the nature of exchangeable cations on LTA-type zeolite hydration. *The Journal of Physical Chemistry C*, 120(40):23254–23261, 2016. DOI:10.1021/acs.jpcc.6b06916 .

[9] Juan José Gutiérrez-Sevillano, Sofía Calero, Said Hamad, Ricardo Grau-Crespo, Fernando Rey, Susana Valencia, Miguel Palomino, Salvador R. G. Balestra, and A. Rabdel Ruiz-Salvador. Critical role of dynamic flexibility in ge-containing zeolites: Impact on diffusion. *Chemistry - A European Journal*, 22(29):10036–10043, jun 2016. DOI:10.1002/chem.201600983 .

[10] J. J. Gutiérrez-Sevillano, S. Calero, S. Hamad, S. R. G. Balestra, R. Grau-Crespo, F. Reya, S. Valencia, and A. R. Ruiz-Salvador. Anomalous breathing behaviour in Ge-LTA zeolite and its implication in enhanced diffusion. In *10th International Symposium on the Characterization of Porous Solids (COPS)*, Mayo 2014. Granada, España.

[11] Said Hamad, Salvador R.G. Balestra, Rocio Bueno-Perez, Sofia Calero, and A. Rabdel Ruiz-Salvador. Atomic charges for modeling metal–organic frameworks: Why and how. *Journal of Solid State Chemistry*, 223:144 – 151, 2015. DOI:10.1016/j.jssc.2014.08.004 . Metal-organic Frameworks-Promising Solid State Porous Materials in 21st Century.

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