

Fecha del CVA	03/10/2019
---------------	------------

Parte A. DATOS PERSONALES

Nombre y Apellidos	Mauricio Rincon Bonilla		
DNI/NIE/Pasaporte		Edad	38
Núm. identificación del investigador	Researcher ID		
	Scopus Author ID		
	Código ORCID	0000-0002-1379-7413	

A.1. Situación profesional actual

Organismo	ASOC BCAM - BASQUE CENTER FOR APPLIED MATHEMATICS		
Dpto. / Centro			
Dirección			
Teléfono	(34) 682381010	Correo electrónico	mrincon@bcamath.org
Categoría profesional	Postdoctoral Research Fellow	Fecha inicio	2017
Espec. cód. UNESCO	221005 - Electroquímica; 221019 - Fenómenos de membrana; 221033 - Fenómenos de transporte; 221108 - Difusión en sólidos		
Palabras clave	Materiales; Estado sólido; Zeolitas y materiales porosos; Nanomateriales		

A.2. Formación académica (título, institución, fecha)

Licenciatura/Grado/Doctorado	Universidad	Año
PhD in Chemical Engineering	The University of Queensland	2014

A.3. Indicadores generales de calidad de la producción científica

Publications: According to the Scopus database, all my papers produced by the date (24) are published in indexed journals ranking in the first quartile (Q1) of different scientific areas, including Material Science, Condensed Matter Physics, Energy, Polymer science, Food Science and Organic Chemistry. Of these, 21 articles are published in scientific journals ranking in the first decile (D1). The lowest and highest impact factor of the Journals I have published in are 3.02 (Materials Open Access) and 8.15 (ACS Applied Materials and Interfaces), respectively. Half of my papers were published after 2015.

According to my Google Scholar profile (<https://scholar.google.com/citations?user=08gly6kAAAAJ&hl=en>), my review in Physical Chemistry Chemical Physics, "Molecular Transport in Nanopores: a Theoretical Perspective", has received 98 citations since 2011. I have a h-index of 12 and have gathered 342 citations.

Outreach: My work has been presented in 6 prestigious international conferences in the areas of Materials Chemistry, Modelling and Simulation, including the AIChE annual meeting, the European Materials Research Society Conference and the Annual Meeting of the Royal Society of Chemistry. This year, I will be presenting my recent work on the simulation of battery materials as an invited speaker at the VIII International Conference on Coupled Problems (on multiscale modelling) and at the special session "EU-Maths-in: Success stories of applications of mathematics in industry" of the 9th International Conference on Industrial and Applied Mathematics.

I have also had the opportunity to reach the general public with my research: my recent collaboration with the Centre for Nutrition and Food Science at the University of Queensland (Australia) on the thermal modelling and characterization of rice-based snacks was showcased in the online science magazine "Mapping Ignorance" (UPV/

EHU) (<https://mappingignorance.org/2018/12/12/is-thermal-sterilisation-of-preservative-free-rice-cakes-possible/>). In addition, the molecular mechanics model of the plant cell wall that I contributed to develop during my collaboration with IBM Research Australia in 2015 led to an animated educational short-film produced by famed science animator Drew Berry (The Walter & Eliza Hall Institute for Medical Research). The film has been shown at biology classes in a number of schools in Melbourne, Australia (<https://www.plantcellwalls.org.au/blog/headlinestory/new-dynamic-computer-models-of-the-plant-cell-wall/>).

Management activities: During my postdoctoral work at Centre of Excellence in Plant Cell Walls (Australia) I was part of the project leadership team, in charge of organizing workshops, an international conferences (the 2014 International Conference in Plant Cell Wall Biology in Australia) and meetings between the different nodes of the Centre. In addition, I have been in charge of the supervision of Internships Masters and PhD students (Rajesh Ranjan, The University of Queensland, 2014; Lachlan Davies, The University of Queensland, 2016; Guo-Dong, BCAM, 2019).

Parte B. RESUMEN LIBRE DEL CURRÍCULUM

I am a Chemical Engineer with ten years of experience in multiscale methods in Computational Material Science, specifically applied to the understanding of diffusion and adsorption in nano and mesoporous materials for industrial and biological applications. I obtained a Ph.D. in Chemical Engineering (2014) from the University of Queensland in Australia (UQ), currently 47th in the QS world university rankings. During my studies under Prof. Suresh Bhatia, I used molecular simulation methods to investigate the suitability of a host of meso and nanoporous materials for the adsorption and separation of fluids in energy storage and molecular sieving applications. This work was validated at the laboratory of Prof. Dr. Jörg Kärger (Leibniz medal recipient) in Leipzig University, Germany, leading to 8 publications in D1 journals and 1 in a Q1 journal.

After my doctorate, I decided to apply my expertise to the study of biological systems and joined the rheology and biolubrication laboratory of Prof. Jason Stokes (UQ), as part of the Centre of Excellence in Plant Cell Walls (a 32 M dollar collaboration between 3 leading Australian Universities and IBM research). In this role, I developed atomistic and continuous models combining diffusion and solid mechanics to unveil the micromechanics of biomaterials such as plant cell walls, articular cartilage and brain tissue. During this period, I was involved in the supervision of several internship students and in multiple teaching activities. In addition, I was part of the Centre leadership team, in charge of the planning and execution of workshops, meetings and an international conference. My work at the Centre and my **continuing collaboration** with its members has led to 12 publications in D1 journals.

In 2017 I returned to the study of inorganic systems when I joined the group of Prof. Elena Akhmatskaya at the Basque Center for Applied Mathematics (BCAM). We are currently working in close collaboration with Dr. J. Carrasco (CIC-energigune, Spain), Prof. J.M. Sanz-Serna (University Carlos III de Madrid, Spain), Prof. S. Bhatia (University of Queensland, Australia) and Prof. F. Jaramillo (Universidad de Antioquia, Colombia) on application of recently proposed in-BCAM enhanced sampling techniques to nanoscale diffusion phenomena in NaFePO₄ cathodes (Na-ion batteries), LLZO solid electrolytes and perovskite-based cathodes (Li-ion batteries). This work has led to 3 articles in D1 Journals and 5 oral presentations in leading international conferences. In 2018 I was awarded the HPC-Europa3 Transnational grant, which allowed me to work with Dr. Tanja van Murik at St Andrews University (UK) for 1.5 months between April and May 2019 on quantum mechanical structural calculations for solid electrolytes in Li-ion batteries. In addition, in 2018 I became a member of the research team of a 300K euros FORMAS grant from the Swedish Research Council (PI is Dr. P. Lopez-Sanchez from the RISE institutes, Sweden) that will investigate food processing in the digestive tract. My role will be devoted to the coarse-grain modelling of the bolus rheology. Finally, I was awarded the prestigious Juan de la Cierva grant (incorporation) from the Spanish Ministry of Science

and Innovation in July 2019, providing 29K euros annually for the development of my research activities in BCAM.

Parte C. MÉRITOS MÁS RELEVANTES (ordenados por tipología)

C.1. Publicaciones

- 1 **Artículo científico.** Akhmatskaya, Elena; et al. 2019. Exploring Li-ion conductivity in cubic, tetragonal and mixed-phase Al-substituted $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ using atomistic simulations and effective medium theory *Acta Materialia*. Elsevier. 175-15, pp.426-435.
- 2 **Artículo científico.** Grace K Dolan; et al. 2018. Probing adhesion between nanoscale cellulose fibres using AFM lateral force spectroscopy: the effect of hemicelluloses on hydrogen bonding *Carbohydrate Polymers*. Elsevier. 208-15, pp.97-107.
- 3 **Artículo científico.** Fabián A García Daza; et al. 2018. Atomistic Insight into Ion Transport and Conductivity in Ga/Al-Substituted $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolytes *ACS applied materials & interfaces*. American Chemical Society. 11-1, pp.753-765.
- 4 **Artículo científico.** L Yu; et al. 2018. New insights into cooked rice quality by measuring modulus, adhesion and cohesion at the level of an individual rice grain *Journal of Food Engineering*. Elsevier. 240, pp.21-28.
- 5 **Artículo científico.** Oliver W Meldrum; et al. 2018. Mucin gel assembly is controlled by a collective action of non-mucin proteins, disulfide bridges, Ca²⁺-mediated links, and hydrogen bonding *Scientific reports*. Nature Publishing Group. 8, pp.5802.
- 6 **Artículo científico.** Mauricio R Bonilla; et al. 2018. Revealing the Mechanism of Sodium Diffusion in Na_xFePO_4 Using an Improved Force Field *The Journal of Physical Chemistry C*. American Chemical Society. 122-15, pp.8065-8075.
- 7 **Artículo científico.** Jing Ai; et al. 2018. Modelling of Thermal Sterilisation of High-Moisture Snack Foods: Feasibility Analysis and Optimization *Food and Bioprocess Technology*. Springer. 11-5, pp.979-990.
- 8 **Artículo científico.** GK Dolan; et al. 2017. Friction, lubrication, and in situ mechanics of poroelastic cellulose hydrogels *Soft Matter*. Royal Society of Chemistry. 13-19, pp.3592-3601.
- 9 **Artículo científico.** Patricia Lopez-Sanchez; et al. 2017. Cellulose-pectin composite hydrogels: Intermolecular interactions and material properties depend on order of assembly *Carbohydrate Polymers*. Elsevier. 162, pp.71-81.
- 10 **Artículo científico.** Gleb E Yakubov; et al. 2017. Mapping nano-scale mechanical heterogeneity of primary plant cell walls *Journal of Experimental Botany*. Oxford University Press. 67-9, pp.2799-2816.
- 11 **Artículo científico.** Patricia Lopez-Sanchez; et al. 2016. Pectin impacts cellulose fibre architecture and hydrogel mechanics in the absence of calcium *Carbohydrate Polymers*. Elsevier. 153, pp.236-245.
- 12 **Artículo científico.** Mauricio R Bonilla; et al. 2016. Micromechanical model of biphasic biomaterials with internal adhesion: Application to nanocellulose hydrogel composites *Acta Biomaterialia*. Elsevier. 29-1, pp.149-160.
- 13 **Artículo científico.** MR Bonilla; et al. 2014. Interpreting atomic force microscopy nanoindentation of hierarchical biological materials using multi-regime analysis *Soft Matter*. Royal Society of Chemistry. 11-7, pp.1281-1292.
- 14 **Artículo científico.** Mauricio Rincon Bonilla; et al. 2014. Understanding Adsorption and Transport of Light Gases in Hierarchical Materials Using Molecular Simulation and Effective Medium Theory *The Journal of Physical Chemistry C*. ACS publications. 18-26, pp.14355-14314.
- 15 **Artículo científico.** P Lopez-Sanchez; et al. 2014. Micromechanics and Poroelasticity of Hydrated Cellulose Networks *Biomacromolecules*. American Chemical Society. 15-6, pp.2274-2284.
- 16 **Artículo científico.** Mauricio Rincon Bonilla; et al. 2013. Diffusion study by IR micro-imaging of molecular uptake and release on mesoporous zeolites of structure type CHA and LTA *Materials*. Multidisciplinary Digital Publishing Institute. 6-7, pp.2662-2688.

- 17 Artículo científico.** Xuechao Gao; et al. 2013. The transport of gases in a mesoporous gamma-alumina supported membrane *Journal of Membrane Science*. Elsevier. 428, pp.357-370.
- 18 Artículo científico.** Mauricio Rincon Bonilla; Suresh K Bhatia. 2013. Diffusion in pore networks: effective self-diffusivity and the concept of tortuosity *The Journal of Physical Chemistry C*. ACS publications. 117, pp.3343-3357.
- 19 Artículo científico.** Xuechao Gao; et al. 2012. The transport of gases in macroporous alpha-alumina supports *Journal of Membrane Science*. Elsevier. 409-410, pp.24-33.
- 20 Artículo científico.** Mauricio R Bonilla; Suresh K Bhatia. 2011. Multicomponent Effective Medium–Correlated Random Walk Theory for the Diffusion of Fluid Mixtures through Porous Media *Langmuir*. ACS publications. 28-1, pp.517-533.
- 21 Artículo científico.** Mauricio Rincon Bonilla; Suresh K Bhatia. 2011. The low-density diffusion coefficient of soft-sphere fluids in nanopores: Accurate correlations from exact theory and criteria for applicability of the Knudsen model *Journal of Membrane Science*. Elsevier. 382-1-2, pp.339-349.
- 22 Artículo científico.** Suresh K Bhatia; Mauricio Rincon Bonilla; David Nicholson. 2011. Molecular transport in nanopores: a theoretical perspective *Physical Chemistry Chemical Physics*. Royal Society of Chemistry. 13-34, pp.15350-15383.
- 23 Artículo científico.** Mauricio Rincon Bonilla; et al. 2010. Heat Treatment-Induced Structural Changes in SiC-Derived Carbons and their Impact on Gas Storage Potential *The Journal of Physical Chemistry C*. ACS Publications. 114-39, pp.16562-16575.
- 24 Artículo científico.** Lopez-Sanchez, P.; et al. Nanostructure and poroviscoelasticity in cell wall materials from onion, carrot and apple: Roles of pectin *Food Hydrocolloids* P.abM.Martinez-SanzacM.R.BonilladF.SonniaE.P.GilbertceM.J.Gidley. 98, pp.105253.

C.2. Proyectos

- 1** Natural texturisers for easy swallowing: Plant polysaccharides role on food swallowability in a biomimetic throat and in vivo Patricia Lopez Sanchez. (Formas: The Swedish Research Council for Environment, Agricultural Sciences and Spatial Planning). 01/01/2019-31/12/2021. 300.000 €. Miembro de equipo.
- 2** Imagenes Electromagneticas del Subsuelo Terrestre Utilizando Metodos Avanzados de Galerkin MICINN (MTM2016-76329-R) David Pardo. (ASOC BCAM - BASQUE CENTER FOR APPLIED MATHEMATICS). 01/01/2017-31/12/2019. Miembro de equipo.
- 3** HPC-Europa3: Transnational Access Programme for a Pan-European Network of HPC Research Infrastructures and Laboratories for scientific computing Mauricio Rincon Bonilla. (Horizon 2020 - European Commission). 07/04/2019-26/05/2019. 3.000 €. Investigador principal.
- 4** CE1101007 Australian Research Council to the ARC Centre of Excellence in Plant Cell Walls Australian Research Council. Vincent Bulone. (University of Adelaide). 01/01/2011-01/01/2017. 12.550.000 €. Miembro de equipo.
- 5** Friction-based modelling of the dynamics of nanoconfined fluid mixtures Australian Research Council. Suresh Bhatia. (The University of Queensland). 01/01/2010-31/12/2014. 650.000 €. Miembro de equipo.

C.3. Contratos

C.4. Patentes