CURRICULUM VITAE (CVA)

CV date	20-06-2024

First name	**Sergio**
Family name	**MADURGA DÍEZ**

Position	Associate Professor (*Professor Agregat*)	
Institution	Universitat de Barcelona (UB)	
Department/Center	Materials Science and Physical Chemistry	Faculty of Chemistry
Country	Spain	
Key words	Monte Carlo simulations, Statistical thermodynamics, Polyelectrolytes, Colloids, Biophysicochemistry	

Sergio Madurga Díez is Associate Professor in the Materials Science and Physical Chemistry Department of Faculty of Chemistry of University of Barcelona.

He obtained a degree in Chemistry from the University of Barcelona in 1998. He pursued a Master's in Physical Chemistry and conducted his doctoral thesis (1999-2003) in the Physical Chemistry Department of the Faculty of Chemistry at the University of Barcelona. In his thesis, he focused on the application and development of molecular simulation techniques. It was evaluated with Excellent Cum Laude, and he received the Extraordinary Doctorate Award from the University of Barcelona.

After that, he undertook a postdoctoral fellowship lasting about two years (2004-2005) at the Research Institute of Biomedicine (IRB). This experience allowed him to apply and develop computer techniques in various biochemical systems of interest.

In September 2005, he joined the Department of Physical Chemistry at the Faculty of Chemistry, University of Barcelona, as a Lecturer for five years in the group of BioPhysicoChemistry of Macromolecules and Colloids (BioPhysChem). Subsequently, he transitioned to the same department as an Associate Professor, serving from 2010 to the present. Currently, he is a member of the Theoretical and Computational Research Institute of UB, which was recently awarded the Maria de Maeztu excellence mention.

He has served as the principal investigator for a University of Barcelona project dedicated to applying new methodologies and teaching strategies to solve chemical problems through computations. Furthermore, he has been the principal investigator of three computational projects in the Red Española de Supercomputación, granted with 133,000, 170,000, and 160,000 computational hours at BSC in 2020, 2021, and 2023, respectively. The first project allowed him to conduct extensive molecular dynamics simulations to understand the pH-dependence of the SARS-Cov-2 main protease. This molecular characterization of the virus target will facilitate the identification of new antiviral drugs. The results have been published in Polymers (2021), 13, 3823. He is engaged in ongoing research to discover small molecules preventing the severe progression of COVID-19 within a project coordinated by Marta Cascante, funded by AGAUR. The second and third computational projects focus on understanding the molecular details of phenylketonuria. Additionally, he has recently

submitted a project utilizing GSMM techniques in a call for the Red Española de Supercomputación (RES), titled 'Integrated Analysis of Metabolic Pathways, Patient Classification, and Knock-Out Strategies in Colorectal Cancer.'

He has supervised the direction of five doctoral theses, covering various topics from Quantum Chemistry applied to the prediction of molecular properties to molecular dynamics of intrinsic disordered proteins (IDP) and the pH effect of biomacromolecules and weak polyelectrolytes. This has led to the development of a set of programs within the group applied to different systems of weak polyelectrolytes. This resource is now accessible to the entire scientific community through the GitHub repository (http://www.github.com/smadurga).
Recently, groundbreaking findings were presented at the EMBO Workshop 2023 titled 'Computational models of life: From molecular biology to digital twins.' This study, which focuses on the impact of cytokine storms in COVID-19, represents cutting-edge research in Genome-Scale Metabolic Models (GSMM) modeling using COBRApy, FBA, Flux Variability Analysis, GIM3E algorithm, and the Metabolic Transformation Algorithm (MTA). The results of the designed workflow are accessible to the community through the GitHub platform.

The main research results and indicators can be summarized as follows: more than 75 research articles (>80% in Q1 by JCR or SJR indexes) and one book and 9 book chapters. H-index of 19 with more than 1500 citations.

Since 2015, Sergio Madurga has been a member of the coordinating committee of the interuniversity master's degree in Atomistic and Multiscale Computational Modeling in Physics, Chemistry, and Biochemistry (UB-UPC), where he coordinates and teaches two subjects. In December 2022, he assumed the role of the general coordinator for this interuniversity UB-UPC master. As the general coordinator of the interuniversity master's degree in Atomistic and Multiscale Computational Modeling, he guides and instructs students, contributing to the future workforce and disseminating knowledge, and is capable of driving technological advancements in various sectors.

He served as a guest editor in Polymers for the Special Issue titled 'Computational Modelling of Biological Processes with Peptides and Proteins' in September 2020. This role enabled him to contribute to the dissemination of knowledge in an open-access format and to advance research in a publicly accessible forum.

Over the past decade, he has been involved in six research transfer projects in collaboration with the Environmental Biotechnology (UB) group led by Prof. Joan Mata and the Integrative Biochemistry (UB) group led by Prof. Marta Cascante, under the coordination of Prof. Francesc Mas. These projects underscore a commitment to tackling real-world challenges through collaborative research, with potential implications for environmental sustainability, biotechnology applications, and advancements in integrative biochemistry that could benefit the broader community.

RELEVANT MERITS.

Publications.

1. Serra-Toro, A.; Vinardell, S.; Astals, S.; **Madurga, S.**; Llorens, J.; Mata-Álvareza, J.; Mas, F.; Dosta, J., “Ammonia recovery from acidogenic fermentation effluents using a gas-permeable membrane contactor”, *Bioresource Technology* **(2022),** 356, 127273. (**Q1, 1st Decile** JCR)

2. Blanco, P.M; **Madurga, S.**; Garcés, J.L; Mas, F.; Dias, R.; “Influence of Macromolecular Crowding in the Charge Regulation of Intrinsically Disordered Proteins”, *Soft Matter* (**2021**), *17*, 655-669. (**Q1** JCR)

3. Nedyalkova, M.; **Madurga, S.**; Tobiszewski, M.; Simeonov, V.; "Calculating the partition coefficients of organic solvents in Octanol/Water and Octanol/Air", *J. Chem. Inf. and Model.* 59, **(2019)** 2257-2263. (**Q1, 1st Decile** Scopus)
4. Blanco, P.M.; **Madurga, S.**; Mas, F.; Garcés, J.L., "Effect of Charge regulation and conformational equilibria in the stretching properties of weak polyelectrolytes", *Macromolecules*, 52 (**2019**), 8017-8031. (**Q1, 1st Decile** JCR)
5. Nedyalkova, M.; Donkova, B.; Romanova, J.; Tzvetkov, G.; **Madurga, S.**; Simeonov, V.; "Iron oxide nanoparticles-In vivo/in vitro biomedical applications and in silico studies". *Advances in Colloid and Interface Science*, 249 **(2017)** 192-212. (**Q1, 1st Decile** Scopus)
6. Hristov, H.; Nedyalkova, M.; **Madurga, S.**; Simeonov, V. "Boron oxide glasses and nanocomposites: synthetic, structural and statistical approach", *J. Mater. Science & Technology*, 33 **(2017)** 535-540. (**Q1, 1st Decile** JCR).

Research projects.

7) 'Unveiling the Phenylalanine coaggregation mechanism for a deep understanding of phenylketonuria disease'. Red Española de Supercomputación. Ref: QH-2023-2-000. 164000 computational hours at BSC. 2023. IP: **Sergio Madurga**.

Contracts, technological or transfer merits,

8) Contract: "Ammonia recovery from animal slurries by means of a novel selective membrane. Stage 1", Company: Indukern-Ravago (Spain), From 2021 to 2022. Import: 88.354,00, IPs: Joan Mata; Francesc Mas

9) Contract: 'Value added products for cosmetic from soybean by-product. Project DIOR'. Company: BUNGE IBERICA SAU (Spain). From: 2018 to 2018. Import: 82.439. IPs: Francesc Mas; Francesc Guardiola; Marta Cascante; Josefa Badia

10) Contract: 'Estudio de laboratorio y planta piloto para la recuperación de amoniaco de los purines. Fase 2' Company: Indukern, S.A. (Spain). From: 2018 to 2018. Import: 17.176. IPs: Joan Mata; Francesc Mas