Luís Mafra, Ph.D. (Resume)

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Domains of expertise: NMR spectroscopy (methods and applications), Materials Science, Physical Chemistry.

Current Position

2014 - Principal Researcher, CICECO – Aveiro Institute of Materials, Univ. of Aveiro, Portugal.

Education

2023-26 Completed course units (18 ECTS) of the B.Sc. in Computer and Informatics Engineering, Univ. of Aveiro: Programming Fundamentals (Python), Introduction to Informatics Engineering, Informatics Laboratories.

2006 Ph.D. in Solid-state NMR Spectroscopy (Physical Chemistry), co-tutelle, CICECO, Univ. of Aveiro, Portugal, and LCS, Univ. of Caen, France.

2003 B.Sc./M.Sc. in Applied Chemistry, Lisbon, Faculty of Sciences and Technology, New Univ. of Lisbon.

Previous Professional Experience

2010-17 Scientific Consultant - Provided consulting services to the pharmaceutical and fertilizer industries.

2012-14 Scientific Consultant - Collaborated on a BP-funded project to investigate zeolite acidity using advanced solid-state NMR techniques.

2007-13 Assistant Researcher, CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal.

2011-12 Invited Professor, University of Oviedo, Spain.

2011 Postdoctoral fellow, Max-Planck Institute for Polymer Research, Mainz, Germany.

2003 Trainee, HOVIONE pharmaceutical company, Loures, Portugal.

Coordination/Participation in R&D Projects & Consulting Activities

- R&D projects sponsored by the petroleum industry:

2012-14 BP Amoco Chemical Company and BP Chemicals, Ltd.
Project: Study of molecular sieve catalysts using solid-state NMR methods

- R&D consulting and advisory for private companies:

2016-17 Hovione Pharma - pharmaceutical company
2016-17 Porcel S.A. - Ceramics Company
2016-18 ZS Pharma, Inc. - AstraZeneca group (San Mateo, CA, USA), team member
2016 ADP Fertilizantes, S.A. (Fertiberia, S.A. group) - fertilizer company
2012 Bial - pharmaceutical company
2010 Nova AP - fábrica de Nitrato de Amónio de Portugal, S.A.
2010 ADP Fertilizantes, S.A. (Fertiberia, S.A. group) - fertilizer company
2010 SOPAC-Sociedade Produtora de Adubos Compostos, S.A. (Fertiberia, S.A. group) - fertilizer company

- Main R&D projects supported by governmental agencies:

Ongoing: PI of **2** R&D projects: an ERC Consolidator Grant (to Nov. 2026) and an FCT India–Portugal bilateral project.
Concluded: PI or Co-PI of **7** R&D projects funded by the European Commission (H2020 INFRAIA PANACEA) and the Portuguese Foundation for Science and Technology; participant in **11** FCT projects.

Scientific Production

- **Publications**: **112** peer-reviewed papers in SCI journals and **6** book chapters, including Nature Commun., JACS, Angew. Chem. Int. Ed., Chem. Mater., Environ. Sci. Technol., ChemSusChem and J. Catal.; h-index 41 (Scopus, October 2026).
- **Presentations**: about **50** invited talks at international conferences, research centres and companies, and **47** contributed talks at international conferences.

Five Selected Scientific Papers

1- Ilkaeva, M., Vieira, R., Pereira, J. M. P., Sardo, M., Marín-Montesinos, I., Mafra, L., Assessing CO_2 capture in porous sorbents via solid-state NMR assisted adsorption techniques, **J. Am. Chem. Soc.**, 145 (**2023**) 8764.

2- Pereira, D., Fonseca, R., Marín-Montesinos, I., Sardo, M., Mafra, L., Understanding CO_2 adsorption mechanisms in porous adsorbents: a solid-state NMR survey, **Curr. Opin. Colloid Interface Sci.**, 64 (**2023**) 101690.

3- Pereira, D., Sardo, M., Marín-Montesinos, I., Mafra, L., One-shot resin 3D-printed stators for low-cost fabrication of magic-angle spinning NMR probeheads, **Anal. Chem.**, 95 (**2023**) 10384.

4- Zelenovskii, P., Soares, M., Bornes, C., Marín-Montesinos, I., Sardo, M., Kopyl, S., Kholkin, A., Mafra, L., Figueiredo, F., Detection of helical water flows in sub-nanometer channels, **Nat. Commun.**, 15 (**2024**) 5516.

5- Mafra, L., Čendak, T., Schneider, S., Wiper, P. V., Pires, J., Gomes, J. R. B., Pinto, M., *The structure of chemisorbed CO_2 species in amine-functionalized mesoporous silicas studied by solid-state NMR and computer modeling*. **J. Am. Chem. Soc.**, 139 (**2017**) 389.

Scientific Recognition & Achievements

Organization of scientific meetings (selected examples)
Co-chaired and organized multiple international and national conferences, including the SMARTER 8 international workshop (2024), the NMR Crystallography Symposium at the 32nd European Crystallographic Meeting (2019), the 2nd National Meeting on Materials Characterization (2016), and the IV Ibero-American NMR Meeting (2012). Chaired notable sessions such as the Nobel Prize session with Kurt Wüthrich (2010).

Institutional roles
Member of the University of Aveiro Disciplinary Committee (since 2015), Manager of the NMR Lab (2007-2023), member of the Portuguese NMR Network (since 2007) and member of the Groupement AMPERE (since 2010).

Editorial, reviewing & expert panels
Evaluated research proposals for various inernational governmental organizations, including ERC, SNSF, CNCS, NSERC, NCN, ISF, and FWO, and served as an expert panelist for ERC grant interviews (2022). Editorial board member for Solid-State NMR (since 2013), Guest Editor for a special issue on NMR Crystallography (2015). Reviewed publications for leading journals such as JACS, ACS Catalysis, and Nature Methods.

Honours & Awards

2024 Univ. Aveiro Researcher Award
2024 SMS Carbon Capture Award
2021 Winning team in the 4th edition of the Blue Bio Value's Ideation
2019 European Research Council (ERC) Consolidator Grant (2 MEur; project 2020-26)
2015 Offered Senior Lecturer position at University of Western Australia (declined)
2014 Adjunct Senior Lecturer honorary title at University of Sydney
2013 FCT Investigator (Portuguese Foundation for Science and Technology): 1 of 74 selected from 1,479 candidates
2012 Research excellence fellowship from Asturias, Spain
2011 CajAstur fellowship at the University of Oviedo, Spain
2011 Max-Planck research fellowship, Mainz, Germany
2009 António Xavier prize - Awarded by Bruker Corp
2006 Celestino da Costa/Jean Perrin Prize
2003-06 FCT doctoral fellowship (Portugal and France)

Skills & Expertise

Scientific and Technical Skills

- NMR Expertise: 20+ years in solid-state NMR spectroscopy, including pulse programming, spectral simulations, method development, and advanced experiments for quadrupolar and spin-1/2 nuclei. Specialized in homonuclear decoupling, inverse detection, and recoupling schemes. My achievements in NMR were recognized with multiple NMR-related prizes and international conference invitations. I highlight the prestigious 2 MEur grant awarded from the European commission solely based on scientific excellence in the NMR field.
- Training & Mentorship: Supervised several undergraduate, Ph.D., and postdoctoral students; delivered NMR courses across Europe.
- Scientific Communication: Proven success in writing project proposals, high-impact publications, and conference presentations.
- Collaboration & Industry Experience: Provided multiple consultancy services and worked on multidisciplinary academic and industrial projects, applying spectroscopy techniques to petroleum, pharmaceutical, and fertilizer industries.
- Additional Expertise: Skilled in analytical complementary characterization methods (e.g., IR/RAMAN spectroscopy, X-ray diffraction, Neutron scattering).

Team Leadership & Management Skills

- **Group leadership:** founded (2020) and lead the SPECKO team, a multidisciplinary group with 2 senior researchers and 1 junior researcher, plus PhD and M.Sc. students, postdocs and fellows; supervised 16 postdoctoral researchers and 10 PhD students.
- **Project and budget management:** PI of an ERC Consolidator Grant (2 MEur); UA PI in the H2020 PANACEA consortium (10 partners); about 6.0 MEur raised as PI or Co-PI; industry contracts as PI.
- **Event organisation and evaluation:** chair of SMARTER 8 (2024) and of the 2012 Ibero-American/GERMN/Iberian NMR meeting; evaluator and panel member for ERC, FWO, ANR, SNSF, NSERC and other funders.

Informatics skills

- OS: Unix (MacOS X, SGI), Linux (Debian, CentOS), Windows, DOS.
- Web & design: Adobe illustrator, CorelDraw, PageMaker, Photoshop, Flash, Fireworks, Ray-tracing software.
- Web CMS software: Apache/IIS + PHP + MySQL open source web platforms.
- Programming / markup languages: Python, Matlab, Unix/Linux shell scripting, LaTeX 2$_\varepsilon$, HTML, XHTML, CSS and some knowledge on C++, java and javascript libraries.
- Computing coursework (Univ. of Aveiro, 18 ECTS): Python, SQL and relational databases, Git, Linux command line, virtual machines and containers, networking basics.

Languages

- Portuguese (native)
- French (native)
- English (C2)
- Spanish (C1)
- German (A1)

Research Interest

My research combines advanced solid-state NMR methodologies with complementary spectroscopies and computational techniques (DFT, AIMD, MLPs) to investigate functional materials. Key areas include: **1)** crystal packing interactions and polymorphic transformations in pharmaceuticals, **2)** the structure and reactivity of acid sites in porous materials (mainly zeolites) relevant to heterogeneous catalysis, and **3)** CO_2 speciation and adsorption mechanisms at the atomic scale in nanoporous materials using pure CO_2, binary mixtures, or industrially relevant gas compositions.

Funding

Since my first R&D project in 2010, I raised a total of about **6.0 Million Eur** as PI or Co-PI (including ~600 kEur from the private sector). From this amount, **2 MEur** were to equip our lab with a DNP-NMR spectrometer in the framework of a strategic national roadmap for research infrastructures. Since 2020, I have also helped to secure about 700 kEur in researcher contracts through competitive calls.

Supervision and Selected Teaching Experience

Ongoing: 2 postdoctoral researchers and 6 PhD students

Concluded: 14 postdoctoral researchers, 3 PhD students (plus 1 discontinued and 3 visiting), 13 M.Sc. students, 3 research fellows and 7 undergraduate projects

- Prepared and taught theoretical and practical NMR courses for international training programmes and NMR schools in Spain, France, Colombia and Brazil, and tutored the national Modern Methods of Structure Elucidation course (IST Lisbon, 2014-21).
- Tutor of the European FAME Master Programme 2014 in the framework of a two years (120 ECTS) Master of Science Program in Advanced Materials Science offered in English by 7 Universities of 4 different countries (France, Germany, Belgium and Portugal)
- Teaching “structural analysis” in the framework of the PhD programme in sustainable chemistry. University of Aveiro, Chemistry Department (2014-21).
- General Chemistry. Second semesters of the 2016 - 2019 academic year, University of Aveiro
- Physical Chemistry. First semester of the 2016-17, 2019-20 academic years, University of Aveiro
- Elements of physical chemistry. First semester of the 2009-2010, 2018-2019 academic years, University of Aveiro