

Website: <http://www.ciceco.ua.pt/luismafra>

Domain of expertise: Solid-state NMR spectroscopy: theory and applications (12 years of experience)

## Education

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- Oct. 2003 - Nov. 2006** Ph.D. awarded by Univ. of Aveiro (Portugal) and Univ. of Caen Normandy (France).  
*Topic:* Theory of solid-state NMR spectroscopy and its application to study materials.
- 1999 - 2003** B.Sc./M.Sc., Applied Chemistry, Lisbon, Faculty of Sciences and Technology, New Univ. of Lisbon (5 years degree).
- 1997 - 1999** Conclusion of the first two years of the B.Sc. in Biotechnology Engineering, Univ. of Algarve, Faro, Portugal.

## Professional Experience

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- Jan. 2014 - present** Promoted to principal Researcher, CICECO-Aveiro Institute of Materials, Univ. of Aveiro, Portugal.
- 2010 - Present** Scientific consulting to the fertilizer industry [*e.g.*, ADP fertilizantes (Fertiberia, S.A. group)].
- Nov. 2012 - Nov. 2014** Consultant of R&D project funded by BP Company to study zeolite acidity using advanced SSNMR methods.
- Dec. 2011 - Dec. 2012** Guest Professor, Univ. of Oviedo, Spain.
- Feb. - Oct. 2011** Invited researcher, Max-Planck Institute for Polymer Research, Mainz, Germany.
- 2007 - 2013** Assistant Researcher, CICECO-Aveiro Institute of Materials, Univ. of Aveiro, Portugal.
- Oct. 2003 - Nov. 2006** Ph.D. fellow at: **1)** Laboratoire de Catalyse et Spectrochimie (LCS), Univ. of Caen Normandy (France) & **2)** CICECO-Aveiro Institute of Materials, Univ. of Aveiro (Portugal).
- Jun. - Oct. 2003** Traineeship at the R&D lab. of HOVIONE pharmaceutical company, Loures, Portugal.
- Summer 2002** ERASMUS traineeship (two months), Univ. of Nottingham, UK.

## Research Interest

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- **Solid-state NMR methodology** - multiple-pulse (CRAMPS-based) methods, fast-MAS methods and sensitivity/resolution enhancement methods for the observation of  $^1\text{H}$  and quadrupolar spins. Use of the GIPAW-DFT approach to calculate NMR tensors in small molecules.
- **Solid-state NMR applications** - Combining high-resolution multinuclear NMR, X-ray diffraction and computer simulations to study packing interactions in pharmaceutical systems (*e.g.*, powdered pharmaceuticals, polymorphism, drug delivery systems); probing acid sites in micro and mesoporous systems relevant to heterogeneous catalysis (*e.g.*, zeolites, silicas and inorganic-organic hybrids); Study of gas-solid interactions in modified porous solid sorbents with potential for gas capture/sorption of gases labeled in key NMR-friendly isotopes.

## Scientific Production

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- **Publications:** Published (or in press) about **63** peer reviewed JCR-indexed papers (from which ~**55%** are found in impact factor (IF) journals IF > 4 (~**40%** at IF > 5, ~**15%** at 4 < IF < 5 and ~**23%** at IF > 7) and **4** book chapters on NMR.
- **Presentations:** Contributed with more than **90** communications in international conferences (including ~**26** talks plus ~**16** “invited talks” at international conferences and **17** invited oral presentations in research centers overseas).

Metrics in WEB OF SCIENCE searching by **AUTHOR:**(mafra l\*) **AND ADDRESS:** (ciceco); or through my **ORCID ID** → <http://orcid.org/0000-0003-1028-8354>

## Coordination & Participation in R&D Projects / Consulting Activities

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- R&D projects sponsored by the petroleum industry:
- Nov. 2012 - Nov. 2014** BP Amoco Chemical Company and BP Chemicals, Ltd. (attracted about 500 k€ for 2 years)  
*Project:* Study of molecular sieve catalysts using solid-state NMR methods.

- R&D consulting and advisory for pharmaceutical and fertilizer companies:

**Jan. 2016 - Jan. 2017** ZS Pharma, Inc. - AstraZeneca group (San Mateo, CA, USA).  
**Jan. 2016** ADP fertilizantes, S.A. (Fertiberia, S.A. group).  
**Apr. 2012** Bial - pharmaceutical company  
**Sep. - Oct. 2010** Nova AP - fábrica de Nitrato de Amónio de Portugal, S.A.  
**May - Oct. 2010** ADP fertilizantes, S.A. (Fertiberia, S.A. group).  
**Apr. - Sept. 2010** SOPAC-Sociedade Produtora de Adubos Compostos, S.A. (Fertiberia, S.A. group.)

- Main R&D projects supported by governmental agencies:

**Concluded:** PI of **3** and participated in **8** R&D projects funded by [the portuguese foundation of science and technology](#).

## Supervision and Teaching Experience

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- Currently supervisor (or co-supervisor) of **2** Post-Docs, **1** PhD student and **1** MSc student.
- Supervised (or co-supervised) **18** researchers: **8** Post-Docs, **3** visiting PhDs, **4** MSc students and **3** grant holders.
- Prepared multiple theoretical and practical NMR courses (about **13**) for European/International training programs and for NMR schools/workshops in countries such as Germany, Brazil, Colombia, Spain, etc.
- Tutor of the European FAME Master Programme 2014 (<http://www.emmi-materials.eu/>) 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 duties in the framework of the PhD program in sustainable chemistry. Supervising the discipline of "structural analysis". **Project:** drug polymorphism, entitled "*Identifying structural features of active pharmaceutical ingredients*", University of Aveiro, Chemistry Department (2013-2016).
- Elements of physical chemistry. First semester of the 2009 - 2010 academic year, University of Aveiro.

## Scientific Recognition & Other Professional Activities

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### Editorial duties:

- Member of the editorial board of "Solid-State NMR" (Elsevier journal).
- Guest-Editor of the special issue "NMR Crystallography" for Solid-State NMR journal.
- Regular reviewer of several Elsevier, Wiley, RSC and ACS journals, including JACS, ACS Catalysis, Chem. Comm. etc.

### Selected scientific & institutional responsibilities

- Invited reviewer by the Czech Science Foundation (the main public funding agency in the Czech Republic) to evaluate project proposals (2016).
- Appointed member of the University Disciplinary Committee (2015).
- Unit manager of the solids NMR lab. at the Univ. of Aveiro (since 2007) and creator of an online web platform to manage routine NMR service.
- Member of the Portuguese NMR network and webmaster of its website (<http://ptnmr.dq.ua.pt>).
- Member of the Organization (or Co-organization) and/or Scientific Committees of 6 international conferences.
- Chairman of the "biosolids & Materials" session @ 1<sup>st</sup> French-Portuguese NMR Conference, Lisbon, Portugal (2016).
- Chair of the IV Ibero-American NMR meeting along with the VI GERMN Bienal and the III Iberian meetings held at the Univ. of Aveiro (2012).
- Coordinator and webmaster of the first national event entitled "NMR & Industry". Univ. of Aveiro, Chemistry Department, Portugal (2010).
- Chairman of the Nobel Prize laureate, Kurt Wüthrich, at the 2<sup>nd</sup> Portuguese Young Chemists Meeting - 2PyChem. Univ. of Aveiro's Rectory, Portugal (2010).

## Honours & Awards

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**2014** Adjunct Senior Lecturer honorary title (Univ. of Sydney, Australia)  
**2013** FCT Investigator award (National Foundation of Science and Technology)  
**2012** Research excellence fellowship for invited Professor (Univ. of Oviedo, Spain)  
**2011** CajAstur fellowship (Univ. of Oviedo, Spain)  
**2011** Max-Planck fellowship (Mainz, Germany)  
**2009** António Xavier prize (Awarded by Bruker Corp.)  
**2006** Celestino da Costa/Jean Perrin Prize (Awarded by APDF - Association of Portuguese Doctors in France)  
**2003 - 2006** Portuguese Foundation of Science and Technology Award  
**2002** Portuguese Ministry of Education Award (mobility grant from Socrates program)