

SHORT CURRICULUM VITAE

Prof. João Rocha

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João Rocha is Full Professor of Chemistry and was Director of the University of Aveiro Institute of Materials-CICECO from 2002 to 2021. At present, he is Coordinator of the Council of Associated Laboratories, a bottom-up organisation gathering the directors of the 40 Associated Laboratories, the main research institutes in the country in all areas of knowledge, representing ca. 10,000 researchers.

Education

Ph.D. in 1990 from the Department of Chemistry, University of Cambridge, UK, working on solid-state NMR of kaolinite and related materials (supervisor Prof. Jacek Klinowski). This was followed by a post-doc (NMR of zeolite-type materials) in the same group. He obtained his 'Agregação' (Habilitation) in 1997 in the University of Aveiro, Portugal.

Honours and Awards

- Officer of the Chemistry Division of the European Academy of Sciences – EURASC (2014), and of the Académie Royal de Belgique des Science, des Lettres et des Beaux-Arts (2022). He is one of the 7 permanent members of the Chemistry Division of the Lisbon Academy of Sciences (created in 1779) since 2006, Fellow of the Royal Society of Chemistry (2016), and Chemistry Europe (2015).
- In 2012-2014, he was advisor for the Prime Minister of Portugal, as a member of the National Science and Technology Council (the only Chemist in this Council).
- He has received from the Portuguese Chemical Society (SPQ) the prizes Alberto Romão Dias (Inorganic and Organometallic Chemistry) in 2021, and Ferreira da Silva (highest SPQ distinction) in 2016; the French-Portuguese prize from the Société Chimique de France (2020); and the Madinabeitia-Lourenço award from the Real Sociedad Española de Química (2015). In 2005, he received the prize for Scientific Excellence from the Portuguese Science Foundation, and in 1990 a prize from Emmanuel College, Cambridge for (for having finished his Ph.D. in two years).
- He coordinated the 2021 and 2023 ERC Consolidator Grants panel PE11 Materials Engineering.

Scientific Record

- Rocha is one of the most cited Portuguese scientists, in all areas. He has published ca. **550 SCI papers and 26 book chapters, with ca. 29,000 citations and Google Scholar h-index 81** (Scopus 24,000 citations, h 72) including in *Nature* and *Nature Nanotechnology* (2), and in the high-impact Chemistry and Materials journals, *viz.*, *Journal of the American Chemical Society* (14), *Angewandte Chemie* (10), *Advanced Materials* (3), *Advanced Functional Materials* (3), *ACS Nano* (3), *Biomaterials* (1), *Chemical Society Reviews* (2), *Coordination Chemistry Reviews* (2), and 5 patent applications. The 2023 ranking by Stanford University and Elsevier places Rocha at the top 1% scientists in all disciplines and in the top 0.2% in Inorganic and Nuclear Chemistry (<https://elsevier.digitalcommonsdata.com/research-data/>). He gave some 300 invited talks at conferences (mostly international). He has mentored 43 post-docs and 36 Ph.D. students.
- He has coordinated over two-dozen projects, which have received >10 M€, including funding by FCT and ANI, and European (as national PI): JOULE(II), 2 Human Capital and Mobility; Materials Network for the Atlantic Area (INTERREG IIIB); ENERMAT, Programme Espace Atlantic, 2007-2013 (INTERREG); Network of Excellence "Functionalized Advanced Materials Engineering of Hybrids and Ceramics (FAME)"; European, COST Action MP1202, "Rational Design of Hybrid Organic-Inorganic Interfaces: the Next Step Towards Advanced Functional Materials", ITN-Marie Skłodowska-Curie Actions, Doctoral Programme IDS-FunMat. Running projects: "Photo-responsive organic-inorganic hybrid multiferroics: A way toward multifunctional electronics", PTDC/CTM-CTM/4044/2020; "Redox-active Metal-Organic Frameworks as Electrode Materials for Lithium-Ion Batteries", PTDC/QUI-ELT/2593/2021. He has consulted widely for industry. He has organized many (inter)national scientific events, the last of which was the "47th IUPAC World Chemistry Congress (Paris, July 2019)". Where he was Member of the Programme Committee, and co-organiser of Symposium T.3: *Hot Topics in Chemistry: a better world through Chemistry*.

Main Scientific Achievements

- Created a field of materials akin to zeolites: microporous silicates of transition metals and lanthanides (over 100 novel Ti, Zr, V, Nb, Cu, Sn, Ca, Y, Ce and other Ln silicates, so-called AV and AM materials) processed in the form of powders, membranes and films. To be clear, these are stoichiometric materials, not metal-doped zeolites, whose archetypal solid is titanium silicate ETS-10 (*Nature*, 367: 347, 1994). He has explored applications in luminescence (*J. Am. Chem. Soc.*, 137:

3051, 2015), catalysis, gas sorption and separation, ion exchange, magnetism and as MRI contrast agents (J. Phys. Chem. B, 1997, 10: 7114, 1997, Eur. J. Inorg. Chem., 801, 2000, J. Am. Chem. Soc., 125: 14573, 2003, Angew. Chem. Int. Ed., 45: 7938, 2006, J. Am. Chem. Soc., 131: 8620, 2009, J. Am. Chem. Soc., 137: 3051, 2015). Outstandingly, one zirconium silicate has found a real commercial application as a drug for the treatment of hyperkalemia.

- Developed unprecedented luminescent lanthanide-bearing Metal Organic Frameworks (MOFs) and coordination polymers (Angew. Chem. Int. Ed., 47: 1080, 2008) and pioneered the field of MOFs nanothermometry (ACS Nano, 7: 7213, 2013, Adv. Funct. Mater., 25: 2824, 2015, Chem. Eur. J., 22: 14782, 2016). Representative other contributions include MOFs transposition of chirality (Inorg. Chem., 51: 1703, 2012), Chem. Commun., 49: 11668, 2013), 2D-3D interconvertible MOFs, and photocatalytic MOFs – Cr(III) and Ag nanoparticles composites (Chem. Eur. J., 21: 11072, 2015).
- Designed a photoresponsive crystalline organic-inorganic hybrid ferroelectric material with a high Curie temperature (423 K), paving the way for accomplishing multiple-state ferroelectric memories, optical switches, and various optoelectronic devices (J. Am. Chem. Soc., 142: 16990, 2020; J. Am. Chem. Soc., 145: 13663, 2023).
- Developed oxide nanoparticles for imaging contrast agents (ACS Nano, 4: 5339, 2010), bimodal imaging (Biomater., 33: 925, 2012), and thermometry (Nature Nanotech, 11: 851, 2016; Adv. Mater., 35: 4868, 2013).
- Designed materials for small-drugs release (including NO, J. Am. Chem. Soc., 133: 6396, 2011).
- Devised materials for a more sustainable World (including anti-mosquito nets, ACS Appl. Mater. Interfaces, 9: 22112, 2017; and uranyl capture Angew. Chem., Intl. Ed., 58: 1, 2019).
- Designed (ca. 40) heterogeneous catalysts based on mesoporous silicas derivatized with metal complexes (J. Mater. Chem., 12: 1735, 2002), and ordered benzene-silica hybrids with molecular-scale periodicity in the walls and different mesopore sizes (J. Mater. Chem., 13:1910, 2003).
- Elucidated the structure of minerals using NMR and XRD techniques (J. Am. Chem. Soc., 113: 7100, 1991; J. Am. Chem. Soc., 114: 6867, 1992; Am. Mineral., 103: 812, 2018).
- Investigated the mechanisms of adsorption and activation of CO₂ on nanoporous materials (Chem. Mater., 23: 1387, 2011).
- Pioneered the development and application of solid-state NMR techniques for studying (i) quadrupolar ($I > 1/2$) nuclei, encompassing ²H exchange NMR (J. Am. Chem. Soc., 114: 6867, 1992), quadrupole nutation and DOR (Solid State NMR, 1: 217, 1992), multiple-quantum MAS NMR and related techniques (FAM MQ MAS, HETCOR MQ MAS, ST MAS, I-ST MAS...) (J. Phys. Chem., 100: 17889, 1996, Solid State NMR, 21: 61, 2002; Magn. Reson. Chem., 41: 679, 2003), and (ii) 1H high-resolution CRAMPS techniques (FSLG, PMLG, DUMBO) (J. Mag. Reson., 199: 111, 2009, Chem. Phys. Lett., 470: 337, 2009). Recent interests include NMR crystallography (Cryst. Growth Design, 13: 2390, 2013) and the development of molecules to probe by NMR microporous solids (J. Am. Chem. Soc., 143: 13616, 2021).

Societal Impact

Rocha is perhaps best known for having extended the realm of zeolitic materials to transition metal and Ln silicate solids. In this context, he developed several microporous zirconium silicates. One such material (AV-13, *Inorg. Chim. Acta*, 356: 19, 2003), slightly modified, was eventually assessed (Rocha was consultant) by the US company ZS Pharma, now part of AstraZeneca, to treat hyperkalemia (excess K⁺ in serum). The new drug *Lokelma* (oral intake) has been approved by FDA and the EMA and is now on the market.

Other Relevant Professional Activities

- Rocha has been in the Chemistry Department, University of Aveiro, since mid 1991 and was promoted to Full Professor of Inorganic Chemistry in 1999. He gave tutorials in Inorganic Chemistry and NMR while at Cambridge. He was invited Professor at Oviedo University in 2010. In Aveiro, he was responsible for courses on Inorganic, and Solid State, Chemistry.
- He was Vice-Director of the European Multifunctional Materials Institute, a follow up of the European Network of Excellence (FAME). He represented Portugal at the ESRF-Grenoble (2004-06) and at the Chairmen of the European Research Councils of Chemistry (2005-07). He was “Secretário Adjunto da Sociedade Portuguesa de Química” (1998-2000).
- He was Chair (and is still a member) of the 'Commission on Inorganic and Mineral Structures' and is consultant of the 'Commission on NMR Crystallography and Related Methods' of the International Union of Crystallography (IUCr). He was editor of the *RSC Nanoscience and Nanotechnology* book series, Chair of the editorial board of *European Journal of Inorganic Chemistry* and was on the editorial board of *Solid State Nuclear Magnetic Resonance*. At present, he is a member of the editorial boards of *Chemistry - a European Journal*, and *Solid-State Sciences*, and editorial advisor for *BMC Chemical Engineering*.
- He has been coordinator and a member of assessment committees of the European Research Council Advanced and Starting Grants (presently coordinates PE11 Materials Engineering), IBM prize Portugal, ANR, LABEX (France), Portuguese Science Foundation (grants and research institutions), and has also reviewed projects and assessed research groups for France, Netherlands, Belgium, Luxembourg, UK, Austria. He is regularly called upon by the Portuguese Science Foundation (FCT) to coordinate the panel awarding post-doc and Ph.D. grants in Materials Science and Engineering, and in 2003 he headed the panel (of foreign scientists) that evaluated the Portuguese Materials Science and Engineering research groups. He has been a regular referee for the leading journals in Chemistry, Materials Science and NMR.

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