

# Curriculum Vitae

**Maria José Calhorda**

## Academic Titles

- Degree in Chemical Engineering (Instituto Superior Técnico, Lisbon, 1979).
- PhD in Chemistry (Instituto Superior Técnico, 1980; Synthesis, characterization and reactivity studies of biscyclopentadienyl derivatives of molybdenum, tungsten and titanium with nitrogen donor ligands).
- "Agregação" in Chemistry (Instituto Superior Técnico, 1993).

## Teaching Activity

- Demonstrator (1969/1971), Teaching Assistant (1971/1980), Assistant Professor (1980-1986), and Associate Professor (1986-1996) at Instituto Superior Técnico (I.S.T.).
- Professor of Inorganic Chemistry at the Department of Chemistry and Biochemistry, Faculty of Science, Universidade de Lisboa, since August 1996.
- Responsible for many undergraduate teaching units in the areas of inorganic and general chemistry, with lectures and laboratories, for Chemistry and Biochemistry students, and several Master teaching units in Chemistry, for Chemistry students (including high school teachers). Participation in doctoral programs.

## Scientific interests

- Current scientific interests are centered around the theoretical study of the electronic structure, properties and reactivity of transition element derivatives in organometallic and inorganic molecules and solids, using ab initio and DFT methods, and including the study of reaction mechanisms (determination of transition states), interpretation of spectra (electronic, vibrational, ESR) and inorganic luminescence. Other areas of activity address the design, synthesis, and characterization of molecular solids based on organometallic molybdenum fragments, and the immobilization of molecules in porous solids (one- and two dimensional) in order to obtain efficient catalysts, as well as to develop metal based antitumor drugs. More recently, the range of complexes has been extended to spin crossover systems (iron and manganese) and the materials to nanoparticles, foams, ionic liquids.

- Post-doctoral studies in the *Inorganic Chemistry Laboratory*, Oxford University, UK, (November 1980 to August 1981), with D.M.P. Mingos; "Visiting Scientist" in *Baker Laboratory*, Department of Chemistry, Cornell University, USA, from September 1987 to September 1988, with R. Hoffmann; Researcher at the Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, from February to October 1995, in the group of A. Simon; Researcher at the University of Marburg, Germany, from May to August 2004, in the group of G. Frenking.

Supervision of undergraduate, Master, PhD, post-doctoral students in research projects; participation in national and international conferences; organization of conferences; scientific referee of several journals (ACS, RSC, Wiley, Elsevier, Springer, Nature Publishing Group). Author or co-author of about 260 scientific papers in peer-reviewed journals (Thomson Reuters), corresponding to a h-index of 38, with 5050 citations (4568 without self-citations, and 19.20 citations per paper; 31 papers of other types; over 250 communications in conferences (invited, oral or poster).

## Other activities

Participation in several committees of the Department of Chemistry and Biochemistry (DQB) and Faculty of Science; Vice-President of the Scientific Council of the Faculty of Science (2002 and 2003); Head of the department (DQB, 2005 and 2006); coordinator of Centro de Química e Bioquímica (unit 612; 2008 and 2009; 2014-); Vice-President of Sociedade Portuguesa de Química (2010-2012); President of Sociedade Portuguesa de Química (2013-2016); Member of Senate of Universidade de Lisboa (elected member of the Commission for Scientific Affairs, since 2013).

## Prizes

Prémio Mobil Oil Portugal, 1970

Prémio Mobil Oil Portugal, 1971

Estímulo à Ciência, Ministério da Ciência e Ensino Superior, 2004

Estímulo à Ciência, Ministério da Ciência e Ensino Superior, 2005

Prémio Alberto Romão Dias, Sociedade Portuguesa de Química, 2011

## Recent Publications (2012-2016)

**TC209** Unveiling the Mechanisms of Catalytic Oxidation Reactions Mediated by Oxo-Molybdenum Complexes: A Computational Overview

M. J. Calhorda, P. J. Costa

*Curr. Org. Chem.* **16**, 2012, 65-72.

**TC210** Electronic structure and properties of camphorimine Cu(I) coordination polymers

M. F. N. N. Carvalho, T. A. Fernandes, A. M. Galvão, N. A. G. Bandeira, M. J. Calhorda, A. M. Botelho do Rego

*J. Pol. Sci. Part A: Pol. Chem.* **50**, 2012, 1102-1110 DOI: 10.1002/pola.25866

**TC211** The influence of crystal packing on *cis-trans* isomerism in nickel(II) complexes with 3-hydroxypicolinic acid and on type of coordination polyhedron in copper(II) complexes

B.-M. Kukovec, P. D. Vaz, M. J. Calhorda, Z. Popović

*Polyhedron* **39**, 2012, 66-75.

**TC212** Syntheses and photophysical properties of new iminopyrrolyl boron complexes and their application in efficient single-layer non-doped OLEDs prepared by spin coating

D. Suresh, C. S. B. Gomes, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita,

M. J. Calhorda, A. Charas, J. Morgado and M. T. Duarte

*Dalton Trans.* **41**, 2012, 8502–8505 DOI: 10.1039/C2DT30487B

**TC213** 1,1'-Bis(diphenylphosphino)ferrocene bridging two mono(cyclopentadienyl) cobalt moieties: synthesis, structure, electrochemistry and DFT studies

V. Rosa, S. Realista, A. Mourato, L. M. Abrantes, J. Henriques, M. J. Calhorda, T. Avilés, M. G. B. Drew, V. Félix

*J. Organomet. Chem.* **712**, 2012, 52-56 DOI: 10.1016/j.jorganchem.2012.04.012

**TC214** An Oligosilsesquioxane Cage Functionalized with Molybdenum(II) Organometallic Fragments

N. L. Dias Filho, F. C. M. Portugal, J. M. F. Nogueira, P. Brandão, V. Félix, P. D. Vaz, Carla D. Nunes, L. F. Veiros, M. J. Villa de Brito, M. J. Calhorda

*Organometallics* **31**, 2012, 4495–4503 <http://dx.doi.org/10.1021/om3003043>.

**TC215** Electronic structure of ytterbium bis -indenyl and -cyclopentadienyl  $\alpha$ -diimines complexes: a DFT and MS-CASPT2 investigation

N. A. G. Bandeira, C. Daniel, A. Trifonov, M. J. Calhorda

*Organometallics* **31** (2012) 4693–4700 DOI: 10.1021/om300081j

**TC216** Photophysical properties of iminopyrrolyl boron complexes: a DFT interpretation

M. J. Calhorda, D. Suresh, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita

*Dalton Trans.* **41**, 2012, 13210 – 13217 DOI:10.1039/C2DT31104F.

**TC217** Charge parametrization of the DvH-c3 heme group: validation using constant-(pH,E) molecular dynamics simulations.

J. Henriques, P. Costa, M. J. Calhorda, M. Machuqueiro

*J. Phys. Chem.* **116**, 2012, 8812 – 8821

**TC218** Tris(organotin)tungstogermanate, a Sandwich Organometallic Derivative of a Keggin type polyoxometalate: Synthesis and DFT study

H. Liu, N. A. G. Bandeira, V. Félix, M. J. Calhorda

*Eur. J. Inorg. Chem.* 2013, 1713 – 1719.

**TC219** Mo(II) complexes of 8-aminoquinoline and their immobilization in MCM-41

M. S. Saraiva, C.D. Nunes, T. G. Nunes, M. J. Calhorda

*J. Appl. Cat. A* **455**, 2013, 172 – 182.

**TC220** Cytotoxicities of Polysubstituted Chlorodicarbonyl(cyclopentadienyl) and (Indenyl)ruthenium Complexes

D. Mavrynsky, J. Rahkila, D. Bandarra, S. Martins, M. Meireles, M.J. Calhorda, I. J. Kovács, I. Zupkó, M. M. Hänninen and R. Leino

*Organometallics* **32**, 2013, 3012-3017.

**TC221** Towards the understanding of radical reactions: experimental and computational studies of titanium(III) diamine bis(phenolate) complexes

S. Barroso, F. Madeira, M. J. Calhorda, M. J. Ferreira, M. T. Duarte and A. M. Martins

*Inorg. Chem.* **52**, 2013, 9427–9439 DOI: 10.1021/ic401008y

**TC222** Self-assembly of copper(II) picolinamide building blocks: synthesis and mechanism

M. Đaković, D. Vila-Viçosa, M. J. Calhorda, N. A. G. Bandeira, B. Kozlevčar, Z. Jagličić, Z. Popović

*Cryst. Eng. Comm.* **15**, 2013, 8074-8087 DOI: 10.1039/C3CE41011K

**TC223** New Mo(II) complexes in MCM-41 and silica: Synthesis and catalysis

M. S. Saraiva, C. I. Fernandes, T. G. Nunes, C. D. Nunes, M. J. Calhorda

*J. Organomet. Chem.* **751**, 2014, 443-452. dx.doi.org/10.1016/j.jorganchem.2013.07.081

**TC224** Unveiling the dual role of the cholinium hexanoate ionic liquid as solvent and catalyst in suberin depolymerisation

R. Ferreira, H. Garcia, A. F. Sousa, M. Guerreiro, F. J. S. Duarte, C. S. R. Freire, M. J. Calhorda, A. J. D. Silvestre, W. Kunz, L. P. N. Rebelo, C. da Silva Pereira

*RSC Adv.* **3**, 2014, 2993-3002. DOI: 10.1039/C3RA45910A, Paper

**TC225** Solvent-Dependent Formation of Os(0) Complexes by Electrochemical Reduction of [Os(CO)(bpy)(L)Cl<sub>2</sub>] (bpy = 2,2'-bipyridine; L = Cl<sup>-</sup>, PrCN)

J. Tory, L. King, A. Maroulis, M. Haukka, M. J. Calhorda and F. Hartl

*Inorg. Chem.* **53**, 2014, 1382-1396. DOI: 10.1021/ic402146t

**TC226** Tunable Fluorophores based on 2-(*N*-Arylimino)pyrrolyl Chelates of Diphenylboron: Synthesis, Structure, Photophysical Characterization and Application in OLEDs

D. Suresh, P. S. Lopes, B. Ferreira, C. A. Figueira, C. S. B. Gomes, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita, M. T. Duarte, A. Charas, J. Morgado, M. J. Calhorda

*Chem. Eur. J.* **20**, 2014, 4126-4140 DOI: 10.1002/chem.201303607

**TC227** Dinuclear Zinc *N*-heterocyclic Carbene Complexes for either the Controlled ROP of lactide or the Controlled Degradation of Polylactide Under Mild Conditions

C. Fliedel, D. Vila-Viçosa, M. J. Calhorda, S. Dagorne, T. Avilés

*ChemCatChem* **6**, 2014, 1357-1367 DOI: 10.1002/cctc.201301015

**TC228** One-Electron Oxidation of ReCp(CO)<sub>2</sub>L (L = PPh<sub>3</sub>, η<sup>2</sup>-2-butene, η-diphenylacetylene): Electrochemical, Spectroscopic and Computational Studies of the Electronic Properties and Dimerization Tendencies of 17-Electron Rhenium Complexes

D. Chong, V. H. Teixeira, M. J. Calhorda, W. E. Geiger

*Organometallics* **33**, 2014, 4706–4715. DOI: 10.1021/om401198j

**TC229** Six-Coordinate High-Spin Iron(II) Complexes with Bidentate PN Ligands based on 2-Aminopyridine – New Fe(II) Spin Crossover Systems

C. Holzhacker, M. J. Calhorda, A. Gil, M. D. Carvalho, L. P. Ferreira, B. Stöger, K. Mereiter, M. Weil, D. Müller, P. Weinberger, E. Pittenauer, G. Allmaier, K. Kirchner  
*Dalton Trans.* **43**, 2014, 11152-11164. DOI: 10.1039/c4dt00186a

**TC230** Successful oxidation of  $\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2$  ( $n = 2, 4, 6$ ) by tellurium leading to  $\text{Ph}_2\text{P}(\text{Te})(\text{CH}_2)_n\text{P}(\text{Te})\text{Ph}_2$

L. Jeremias, M. Babiak, V. Kubát, M.J. Calhorda, Z. Trávníček, J. Novosad  
*RSC Adv.* **4**, 2014, 15428-15430. DOI: 10.1039/C4RA00157E, Communication

**TC231** CNN Pincer Ruthenium Catalysts for Transfer and  $\text{H}_2$  Hydrogenation of Ketones: Experimental and Computational Studies

W. Baratta, M. J. Calhorda, P. J. Costa, G. Esposito, E. Herdtweck, S. Magnolia, C. Mealli, A. Messaoudi, S. A. Mason, L. F. Veiros  
*Chem. Eur. J.* **20**, 2014, 13603-13617 DOI: 10.1002/chem.201402229

**TC232** Four- and five-coordinate high-spin iron(II) complexes bearing bidentate soft/hard SN ligands based on 2-aminopyridine

C. Holzhacker, M. J. Calhorda, A. Gil, M. D. Carvalho, L. P. Ferreira, K. Mereiter, B. Stöger, E. Pittenauer, G. Allmaier, K. Kirchner  
*Polyhedron* **81**, 2014, 45–55. <http://dx.doi.org/10.1016/j.poly.2014.05.052>

**TC233** Cationic Half-Sandwich Iron(II) and Iron(III) Complexes with N-Heterocyclic Carbene Ligands

J.M.S. Cardoso, A. Fernandes, B.P. Cardoso, M.D. Carvalho, L.P. Ferreira, M.J. Calhorda, B. Royo  
*Organometallics* **33**, 2014, 5670–5677. DOI: 10.1021/om500528p

**TC234** Influence of activated carbons porous structure on iopamidol adsorption

A. S. Mestre, M. Machuqueiro, M. Silva, R. Freire, I. M. Fonseca, M. S. C. S. Santos, M. J. Calhorda, A. P. Carvalho  
*Carbon* **81**, 2014, 607-615. [doi.org/10.1016/j.carbon.2014.05.065](http://doi.org/10.1016/j.carbon.2014.05.065)

**TC235** Synthesis, Cytotoxic and Hydrolytic Studies of Titanium Complexes Anchored by a Tripodal Diamine Bis(phenolate) Ligand

S. Barroso, A.M. Coelho, S. Gómez-Ruiz, M.J. Calhorda, Ž. Žižak, G. N. Kaluderović, A.M. Martins  
*Dalton Trans.* **43**, 2014, 17422–17433 DOI: 10.1039/C4DT00975D

**TC236** Vanadyl cationic complexes as catalysts in olefin oxidation

C. D. Nunes, P.D. Vaz, V. Félix, L. F. Veiros, T. Moniz, M. Rangel, S. Realista, A. C. Mourato, M. J. Calhorda  
*Dalton Trans.* **44**, 2015, 5125–5138 DOI: 10.1039/C4DT03174A

**TC237** Pore size matters! Helical heterogeneous catalysts in olefin oxidation

M.S. Saraiva, C.I. Fernandes, T.G. Nunes, M.J. Calhorda, C.D. Nunes  
*Appl. Catal. A* **180**, 2015, 130–140 [dx.doi.org/10.1016/j.apcata.2015.01.040](http://dx.doi.org/10.1016/j.apcata.2015.01.040)

**TC238** Molybdenum(II) catalyst precursors in olefin oxidation reactions

C.D. Nunes, M. J. Calhorda  
*Inorg. Chim. Acta* **431**, 2015, 122–131 <http://dx.doi.org/10.1016/j.ica.2015.03.018>

**TC239** Fe(III) SalEen derived Schiff base complexes as potential contrast agents

B. P. Cardoso, A. I. Vicente, J. B. J. Ward, P. J. Sebastião, F. V. Chávez, S. Barroso, A. Carvalho, S. J. Keely, P. N. Martinho, Maria José Calhorda

**TC240** Asymmetric Binuclear Ni(II) And Cu(II) Schiff Base Metallopolymers

S. Realista, A. S. Viana, B. P. Cardoso, A. M. Botelho do Rego, P. D. Vaz, A. I. Melato, P. N. Martinho, M. J. Calhorda  
*RSC Adv.* **5**, 2015, 39495-39504

**TC241** Comparing spectroscopic and electrochemical properties of complexes of type  $[\text{Cp}'\text{M}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2]$  ( $\text{Cp}' = \text{Cp}$ , Ind, Flu;  $\text{M} = \text{Mo}$ , W): a complementary experimental and DFT study

I. S. Gonçalves, L. F. Veiros, C. A. Gamelas, C. Cabrita, M. J. Calhorda, C. F. G. C. Geraldès, J. Green, E. Packham, M. G. B. Drew, V. Félix, A. G. Santos, C. C. Romão  
*J. Organomet. Chem.* **792**, 2015, 154-166 [dx.doi.org/10.1016/j.jorganchem.2015.04.001](http://dx.doi.org/10.1016/j.jorganchem.2015.04.001)

**TC242** Preference for sulfoxide S- or O-bonding to 3d transition metals – DFT insights

B.P. Cardoso, B. Royo, M. J. Calhorda  
*J. Organomet. Chem.* **792**, 2015, 167-176 [dx.doi.org/10.1016/j.jorganchem.2015.04.022](http://dx.doi.org/10.1016/j.jorganchem.2015.04.022)

**TC243** Catalytic activity of Mo(II) complexes in homogeneous and heterogeneous conditions

Maria Vasconcellos Dias, Marta S. Saraiva, Paula Ferreira, and Maria José Calhorda  
*Organometallics* **34**, 2015, 1465-1478 [doi: 10.1021/om501068q](https://doi.org/10.1021/om501068q)

**TC244** Luminescent Di- and Trinuclear Boron Complexes Based on Aromatic

Iminopyrrolyl Spacer Ligands: Synthesis, Characterization and Application in OLEDs  
D. Suresh, C. S. B. Gomes, P. S. Lopes, C. A. Figueira, B. Ferreira, P. T. Gomes, R. E. Di Paolo, A. L. Maçanita, M. T. Duarte, A. Charas, J. Morgado, D. Vila-Viçosa, M. J. Calhorda  
*Chem. Eur. J.* **21**, 2015, 9133-9149 DOI: 10.1002/chem.201500109

**TC245** How the Intercalation of Phenanthroline Affects the Structure, Energetics and Bond Properties of DNA Base Pairs. Theoretical Study Applied to Adenine-Thymine and Guanine-Cytosine Tetramers

A. Gil, V. Branchadell, M.J. Calhorda  
*J. Chem. Theory Comput.* **11**, 2015, 2714–2728 DOI: 10.1021/ct5006104

**TC246** Synthesis and Reactivity of Taddol-Based Chiral Fe(II) PNP Pincer Complexes - Solution Equilibria between  $\kappa^2\text{P,N-}$  and  $\kappa^3\text{P,N,P-}$  Bound PNP Pincer Ligands

C. Holzhaecker, B. Stöger, M. D. Carvalho, L. P. Ferreira, E. Pittenauer, G. Allmaier, L. F. Veiros, S. Realista, A. Gil, M. J. Calhorda, D. Müller, K. Kirchner  
*Dalton Trans.* **44**, 2015, 13071–13086

**TC247** Wittig Reaction: Domino Olefination and Stereoselectivity DFT Study. Synthesis of the Miharamycins' Bicyclic Sugar Moiety

V. Cachatra, A. Almeida, J. Sardinha, S. D. Lucas, A. Gomes, P. D. Vaz, M. H. Florêncio, R. Nunes, D. Vila-Viçosa, M. J. Calhorda, A. P. Rauter  
*Org. Lett.* **17**, 2015, 5622–5625. DOI: 10.1021/acs.orglett.5b02849

**TC248** Mechanistic Study of the Direct Intramolecular Allylic Amination Reaction Catalyzed by Palladium(II)

F. J. S. Duarte, G. Poli, M. J. Calhorda  
*ACS Cat.* **6**, 2016, 1772–1784 DOI: 10.1021/acscatal.5b02091

**TC249** Reaction of  $\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2$  ( $n = 1, 3, 5$ ) with elemental tellurium and comparison with members of even-numbered series

L. Jeremias, M. Babiak, V. Kubát, M.J. Calhorda, Z. Trávníček, J. Novosad  
*Inorg. Chim. Acta.* **443**, 2016, 230-234. [doi:10.1016/j.ica.2016.01.015](https://doi.org/10.1016/j.ica.2016.01.015)

**TC250** Opening the Way to Catalytic Aminopalladation/Proxycyclic Dehydropalladation:

Access to Methylidene  $\gamma$ -Lactams

M. M. Lorion, F. J. S. Duarte, M. J. Calhorda, J. Oble, G. Poli

*Org. Letters*, **18**, 2016, 1020–1023

DOI: 10.1021/acs.orglett.6b00143

**TC251** Dynamic spin interchange in a tridentate Fe(III) Schiff-base compound

A.I. Vicente, A. Joseph, L. P. Ferreira, M. Deus Carvalho, V. H. N. Rodrigues, M. Duttine, H.

P. Diogo, M. E. M. Piedade, M. J. Calhorda, P. N. Martinho

*Chem. Sci.* **7**, 2016, 4251–4258.

DOI: 10.1039/C6RA12026A

**TC252** Helical materials with chiral Mo(II) catalysts

M. S. Saraiva, C. I. Fernandes, T. G. Nunes, C. D. Nunes, M. J. Calhorda

*Topics Catal.* **59**, 2016, 1237–1248.

DOI 10.1007/s11244-016-0644-5

**TC253** A Mn(III) single ion magnet with tridentate Schiff-base ligands

S. Realista, A. J. Fitzpatrick, G. Santos, L. P. Ferreira, S. Barroso, L. C. J. Pereira, N. A. G.

Bandeira, P. Neugebauer, J. Hrubý, G. G. Morgan, J. van Slageren, M. J. Calhorda, P. N.

Martinho

*Dalton Trans.* **45**, 2016, 12301–12307.

DOI: 10.1039/C6DT02538B, Communication

**TC254** Boron complexes of aromatic ring fused iminopyrrolyl ligands: synthesis, structure, and luminescence properties

D. Suresh, B. Ferreira, P. S. Lopes, C. S. B. Gomes, P. Krishnamoorthy, A. Charas, D. Vila-

Viçosa, J. Morgado, M. J. Calhorda, A. L. Maçanita, P. T. Gomes

*Dalton Trans.* **45**, 2016, 15603–15620.

DOI: 10.1039/C6DT02771G, Paper

**TC255** Heterodinuclear Ni(II) and Cu(II) Schiff base complexes and their activity in oxygen reduction

S. Realista, P. Ramgi, B. P. Cardoso, A. I. Melato, A. S. Viana, M. J. Calhorda, P. N. Martinho

*Dalton Trans.* **45**, 2016, 14725–14733.

DOI: 10.1039/C6DT01903J

**TC256** Di- versus Trinuclear Copper(II) Cryptate for the Uptake of Dicarboxylate Anions

C. V. Esteves, P. Mateus, V. André, N. A. G. Bandeira, M. J. Calhorda, L. P. Ferreira, R.

Delgado

*Inorg. Chem.* **55**, 2016, 7051–7060.

DOI: 10.1021/acs.inorgchem.6b00945

**TC257** Porous materials as delivery and protective agents for Vitamin A

I. Calabrese, M. L. Turcoliveri, M. J. Ferreira, A. Bento, P. D. Vaz, M. J. Calhorda, C. D. Nunes

*RSC Adv.* **6**, 2016, 66495–66504.

DOI: 10.1039/C6RA12026A

**TC258** New heterogeneous catalysts with Mo(II) intercalated in layered double hydroxides

M. Diaz-Couce, J. Marreiros, M. J. Ferreira, P. D. Vaz, C. D. Nunes, M. J. Calhorda

*Inorg. Chim. Acta* **##**, 2016, ##-##.

<http://dx.doi.org/10.1016/j.ica.2016.07.030>

**TC259** A Theoretical Study of Methylation and CH/ $\pi$  Interactions in DNA Intercalation:

Methylated 1,10-Phenanthroline in Adenine-Thymine Base Pairs

A. Gil, V. Branchadell, M. J. Calhorda

*RSC Adv.* **6**, 2016, 85891–85902.

DOI: 10.1039/C6RA15495F, Paper

**TC260** Electrochemical studies and potential anticancer activity in Ferrocene derivatives

S. Realista, S. Quintal, P. N. Martinho, A. I. Melato, A. Gil, T. Esteves, M. D.

Carvalho, L. Ferreira, P. D. Vaz, M. J. Calhorda

*J. Coord. Chem.* (accepted)