Jorge Manuel Campos Marques

CURRICULUM VITÆ

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Name: Jorge Manuel Campos Marques
Affiliation: José António de Almeida Marques, and Adelaide da Costa Campos Marques
Place of born: Lajeosa, Tondela (Viseu), Portugal
Date of born: 6th of July, 1968

Academic degrees

1987: Secondary School with the classification of 17 out of 20.
1991: Graduation in Chemistry by the University of Coimbra with the classification of 16 out of 20.
1995: PhD in Theoretical Chemistry by the University of Coimbra with the highest classification.

Scientific activities

Fellowships and thesis

1990-91: Young Researchers Grant from Instituto Nacional de Investigação Científica (INIC) to begin the theoretical dynamics study of the O + OH reaction, under supervision of Prof. A.J.C. Varandas.
1991-95: PhD fellowship from Junta Nacional de Investigação Científica e Tecnológica (JNICT), under Programmes CIÊNCIA and PRAXIS XXI. The theoretical work on elementary reactions and the problem of the zero-point energy in classical dynamics, under supervision of Prof. A.J.C. Varandas, is the basis of the PhD thesis entitled "Colisões moleculares em sistemas reactivos e o problema da energia de ponto-zero em dinâmica clássica". The monography "Caos determinístico em sistemas Hamiltonianos" about deterministic chaos has also been presented.

Research projects

Principal investigator of the following projects:

1. "Theoretical and computational studies of dissociation reactions occurring in hyperthermal conditions: from small ionic systems to clusters", financed by Fundação para a Ciência e Tecnologia (PTDC/QUI/69422/2006), 2009-2012.

2. "Dinâmica Clássica e Semi-clássica em Sistemas Reactivos", J.M.C. Marques (leader of the portuguese team) and S.A. Vázquez (leader of the spanish team). "Acção Integrada Luso-Espanhola" financed by both Conselho de Reitores das Universidades Portuguesas (E-10/03), Portugal, and Ministerio de Ciencia y Tecnología (HP2002-0071), Spain,

3. "Potential energy surfaces and global minima search on van der Waals and ion microsolvated clusters", provision of supercomputer time at the John von Neumann Institut für Computing, Jülich, Germany (Project EPG010), 2006-2010.

4. "Estudos das paisagens energéticas de agregados atómicos utilizando algoritmos de inspiração biológica inovadores", bilateral project financed by FCT, Portugal, and CAPES, Brazil (Project: FCT-2984/CAPES-8607/14-1), 2016-2018. This a joint project with the group of Prof. Frederico Prudente (Universidade Federal da Bahia, Brazil).

Team member in the following projects:

1. "Theoretical and Computational Studies of Elementary Reactions with Relevance in Atmospheric Chemistry and Combustion Processes", financiado pela Fundação para a Ciência e Tecnologia sob os programas PRAXIS XXI e FEDER (contracto 2/2.1/QUI/408/94).

2. "Theory and Computation of Chemical Reactions. From Fundamental Aspects to Applications with Relevance in Environmental Chemistry", financiado pela Fundação para a Ciência e Tecnologia (PRAXIS/P/QUI/10000/1998).

3. "Electronic Structure and Dynamics of Reactive Molecules: From Fundamental Issues to Applications in Environmental Chemistry, Astrophysics and Catalysis", financiado pela Fundação para a Ciência e Tecnologia (POCTI/QUI/40154/2001).

4. "Quantum chemistry within the Born-Oppenheimer aproximation and beyond: From first principles to predicting capability", financiado pela Fundação para a Ciência e Tecnologia (POCI/QUI/60501/2004).

5. "Development of New Evolutionary Computation Approaches for Applications in Theoretical Chemistry", financiado pela Fundação para a Ciência e Tecnologia (POSC/EIA/55951/2004).

6. "Química Teórica Ambiental", financiado pela Fundação para a Ciência e Tecnologia (POCI/AMB/60261/2004).

7. "Química Computacional com relevância na atmosfera, astrofísica e catálise", financiado pela Fundação para a Ciência e Tecnologia (REEQ/128/QUI/2005).

8. ""Interactions in polyelectrolyte complexes: simulation and experiment", financed by Fundação para a Ciência e Tecnologia (PTDC/QUI-QUI/101442/2008).

9. "High-Performance Computing over the Large-Scale Internet", financed by Fundação para a Ciência e Tecnologia (PTDC/EIA-EIA/102212/2008).

10. "Molecules in motion (MOLIM)", Chemistry and Molecular Sciences and Technologies, COST Action CM1405, supported by the EU Framework Programme Horizon 2020, 2015-2019.

11. "How to protect water, soil and plants production all together", financed by Fundação para a Ciência e Tecnologia (WaterJPI/0006/2016), 2017-2020.

Publications

1. "A detailed state-to-state low-energy dynamics study of the reaction $O(^3P) + OH(^2\Pi) \rightarrow O_2(\tilde{X}^3\Sigma_g^-) + H(^2S)$ using a quasiclassical trajectory-internal-energy quantum-mechanical-threshold method"
   A.J.C. Varandas and J.M.C. Marques, *J. Chem. Phys.* **97**, 4050-4065 (1992).

2. "QCT-IEQMT calculations of the $O(^3P) + OD(^2\Pi)$ reaction at low energies"
   J.M.C. Marques and A.J.C. Varandas, *An. Fis.* **90**, 284-292 (1994).

3. "Method for quasiclassical trajectory calculations on potential energy surfaces defined from gradients and Hessians, and model to constrain the energy in vibrational modes"
   A.J.C. Varandas and J.M.C. Marques, *J. Chem. Phys.* **100**, 1908-1920 (1994).

4. "Dynamics calculations and isotopic effect in $O + OH(D) \rightarrow O_2 + H(D)$ at low energies"

J.M.C. Marques, W. Wang and A.J.C. Varandas, *J. Chem. Soc. Faraday Trans.* **90**, 2189-2200 (1994).

5. "Estudos teóricos de reacções químicas elementares: da energética à dinâmica"
   A.J.C. Varandas, A.A.C.C. Pais and J.M.C. Marques, *Colóquio sobre Termodinâmica e Reactividade de Sistemas Moleculares* (Academia das Ciências de Lisboa, Lisboa, 1994), p.197-234.

6. "On the chaperon mechanism for association rate constants: the formation of HO_2 and O_3"
   A.J.C. Varandas, A.A.C.C. Pais, J.M.C. Marques and W. Wang, *Chem. Phys. Lett.* **249**, 264-271 (1996).

7. "Dynamics study of the $H + ArO_2$ multichannel reaction"
   J.M.C. Marques, W. Wang, A.A.C.C. Pais e A.J.C. Varandas, *J. Phys. Chem.* **100**, 17513-17522 (1996).

8. "Classical trajectory study of mode specificity and rotational effects in unimolecular dissociation of HO_2"
   J.M.C. Marques and A.J.C. Varandas, *J. Phys. Chem. A* **101**, 5168-5173 (1997).

9. "Trajectory surface hopping study of $Li + Li_2\,(X^1\Sigma_g^+)$ dissociation reaction"
   A.I. Voronin, J.M.C. Marques and A.J.C. Varandas, *J. Phys. Chem. A* **102**, 6057-5173 (1998).

10. "Comparative trajectory surface hopping study for the $Li + Li_2\,(X^1\Sigma_g^+)$, $Na + Li_2\,(X^1\Sigma_g^+)$ and $Li + Na_2\,(X^1\Sigma_g^+)$ dissociation reactions"
    J.M.C. Marques, A.I. Voronin and A.J.C. Varandas, *Phys. Chem. Chem. Phys.* **1**, 2657-2665 (1999).

11. "Mode specificity study in unimolecular dissociation of nonrotating H_2O, DHO, and MuHO molecules"
    J.L. Llanio-Trujillo, J.M.C. Marques and A.J.C. Varandas, *J. Phys. Chem. A* **103**, 10907-10914 (1999).

12. "Isotope effect on unimolecular dissociation of MuO_2: a classical trajectory study"
    J.M.C. Marques, J.L. Llanio-Trujillo and A.J.C. Varandas, *Phys. Chem. Chem. Phys.* **2**, 3583-3589 (2000).

13. "On the high pressure rate constants of the H/Mu + O_2 addition reactions"
J.M.C. Marques and A.J.C. Varandas, *Phys. Chem. Chem. Phys.* **3**, 505-507 (2001).

14. "Reply to the Comment on 'On the high pressure rate constants of the H/Mu+ O_2 addition reactions' by L.B. Harding, J. Troe and V.G. Ushakov, Phys. Chem. Chem. Phys., 2001, 3, 2030"
J.M.C. Marques and A.J.C. Varandas, *Phys. Chem. Chem. Phys.* **3**, 2632-2633 (2001).

15. "A direct dynamics study of the H_2 elimination from 2,5-dihydrofuran"
E. Martínez-Núñez, J.M.C. Marques and S.A. Vázquez, *J. Chem. Phys.* **115**, 7872-7880 (2001).

16. "Li+Li_2 dissociation reaction using the self-consistent potential and trajectory surface hopping methods"
J.M.C. Marques, A.I. Voronin and A.J.C. Varandas, *J. Phys. Chem. A* **106**, 3673-3080 (2002).

17. "Dynamics calculations for the Cl + C_2H_6 abstraction reaction: Thermal rate constants and kinetic isotope effects"
A. Fernández-Ramos, E. Martínez-Núñez, J.M.C. Marques and S.A. Vázquez, *J. Chem. Phys.* **118**, 6280-6288 (2003).

18. "Time dependent wave packet study of the electronically non-adiabatic Cl+H_2 reaction using a one-dimensional model"
F.V. Prudente, A. Riganelli and J.M.C. Marques, *Phys. Chem. Chem. Phys.* **5**, 2354-2359 (2003).

19. "O método das trajectórias clássicas: colisões coplanares do tipo A+BC"
J.M.C. Marques, A. Riganelli and A.J.C. Varandas, *Quim. Nova* **26**, 769-778 (2003).

20. "Dynamics study of ClO + O_2 collisions and their role in the chemistry of stratospheric ozone"
O.B.M. Teixeira, J.M.C. Marques and A.J.C. Varandas, *Phys. Chem. Chem. Phys.* **6**, 2179-2184 (2004).

21. "Quasiclassical trajectory study of the collision-induced dissociation of CH_3SH^++ Ar"
E. Martínez-Núñez, S.A. Vázquez and J.M.C. Marques, *J. Chem. Phys.* **121**, 2571-2577 (2004).

22. "Trajectory dynamics study of the Ar + CH_4 dissociation reaction at high temperatures: the importance of zero-point-energy effects"
J.M.C. Marques, E. Martínez-Núñez, A. Fernández-Ramos and S.A. Vázquez, *J. Phys. Chem. A* **109**, 5415-5423 (2005).

23. "Quasiclassical dynamics simulation of the collision-induced dissociation of $Cr(CO)_6^+$ with Xe"
E. Martínez-Núñez, A. Fernández-Ramos, S.A. Vázquez, J.M.C. Marques, M. Xue, and W.L. Hase, *J. Chem. Phys.* **123**, 154311 (2005).

24. "Trajectory dynamics study of collision-induced dissociation of the Ar + CH_4 reaction at hyperthermal conditions: vibrational excitation and isotope substitution"
J.M.C. Marques, E. Martínez-Núñez and S.A. Vázquez, *J. Phys. Chem. A* **110**, 7113-7121 (2006).

25. "Analysis of locality in hybrid evolutionary cluster optimization"
F.B. Pereira, J.M.C. Marques, T. Leitão, and J. Tavares, *Proceedings of the 2006 IEEE Congress on Evolutionary Computation*, Vols. 1-6, p. 2270-2277, CEC, Vancouver, Canada, 2006.

26. "Kinetics and dynamics of O + OClO reaction in a modified many-body expansion potential energy surface for ClO_3"
O.B.M. Teixeira, J.M.C. Marques and A.J.C. Varandas, *Int. J. Chem. Kinet.* **39**, 422-430 (2007).

27. "Symmetry numbers and chemical reaction rates"
A. Fernández-Ramos, B.A. Ellingson, R. Meana-Pañeda, J.M.C. Marques and D.G. Truhlar, *Theor. Chem. Acc.* **118**, 813-826 (2007).

28. "Designing efficient evolutionary algorithms for cluster optimization: a study on locality"
F.B. Pereira, J.M.C. Marques, T. Leitão, and J. Tavares, in *Advances in Metaheuristics for Hard Optimization*, P. Siarry and Z. Michalewicz (Eds.), Springer, 2008; p. 223-250.

29. "A Quantum Mechanics Toolkit: Useful Internet Toolkit to Teach Fundamental Concepts of Quantum Mechanics"
J.P.M. Poiares, S.P.J. Rodrigues, and J.M.C. Marques, *J. Chem. Educ.* **85**, 591 (2008).

30. "A new genetic algorithm to be used in the direct fit of potential energy curves to *ab initio* and spectroscopic data"
J.M.C. Marques, F.V. Prudente, F.B. Pereira, M.M. Almeida, A.M. Maniero, and C.E. Fellows, *J. Phys. B: At., Mol. & Opt. Phys.* **41**, 085103 (2008).

31. "On the Use of Different Potential Energy Functions in Rare-Gas Cluster Optimization by Genetic Algorithms: Application to Argon Clusters"
J.M.C. Marques, F.B. Pereira, and T. Leitão, *J. Phys. Chem. A* **112**, 6079-6089 (2008).

32. "A Hybrid Evolutionary Algorithm for Cluster Geometry Optimization: the importance of structural elitism",
F.B. Pereira and J.M.C. Marques, *Proceedings of the Eighth International Conference on Hybrid Intelligent Systems (HIS 2008)*, p. 911-914, IEEE Computer Society, Los Alamitos, CA, USA, 2008.

33. "A Self-Adaptive Evolutionary Algorithm for Cluster Geometry Optimization",
F.B. Pereira and J.M.C. Marques, *Proceedings of the Eighth International Conference on Hybrid Intelligent Systems (HIS 2008)*, p. 678-683, IEEE Computer Society, Los Alamitos, CA, USA, 2008.

34. "Time-dependent wave packet calculation of the LiH + H reactive scattering on a new potential energy surface", F.V. Prudente, J.M.C. Marques, and A.M. Maniero, *Chem. Phys. Lett.* **474**, 18-22 (2009).

35. "A study on diversity for cluster geometry optimization",
F.B. Pereira and J.M.C. Marques, *Evol. Intel.* **2**, 121-140 (2009).

36. "An evolutionary algorithm for global minimum search of binary atomic clusters",
J.M.C. Marques and F.B. Pereira, *Chem. Phys. Lett.* **485**, 211-216 (2010).

37. "Transport Properties of Aqueous Solutions of (1R,2S)-(-)- and (1S,2R)-(+)-Ephedrine Hydrochloride at Different Temperatures",
A.J.M. Valente, A.C.F. Ribeiro, J.M.C. Marques, P.E. Abreu, V.M.M. Lobo, and K. Kataky, *J. Chem. Eng. Data* **55**, 1145-1152 (2010).

38. "Generation and Characterization of Low-Energy Structures in Atomic Clusters",
J.M.C. Marques, A.A.C.C. Pais, and P.E. Abreu, *J. Comput. Chem.* **31**, 1495-1503 (2010).

39. "How different are two chemical structures?",
J.M.C. Marques, J.L. Llanio-Trujillo, P.E. Abreu, and F.B. Pereira *J. Chem. Inf. Model.* **50**, 2129-2140 (2010).

40. "Towards an effective evolutionary approach for binary Lennard-Jones clusters",
F.B. Pereira and J.M.C. Marques, *Proceedings of the 2010 IEEE Congress on Evolutionary Computation*, p. 1-7, CEC, Barcelona, Spain, 2010.

41. "Analysis of Crossover Operators for Cluster Geometry Optimization",
F.B. Pereira and J.M.C. Marques, in *Computational Intelligence for Engineering Systems: Emergent Applications, Intelligent Systems, Control and Automation, Science and Engineering Series*, Vol. 46, A. Madureira, J. Ferreira and Z. Vale (Eds.), Springer-Verlag, 2011; p. 77-89.

42. "An Evolutionary Algorithm for the Global Optimization of Molecular Clusters: Application to Water, Benzene, and Benzene Cation",
J.L. Llanio-Trujillo, J.M.C. Marques, and F.B. Pereira *J. Phys. Chem. A* **115**, 2130-2138 (2011).

43. "Electronic structure calculations on the Ar-C_6H_{12} interaction: application to the microsolvation of the chair conformer",
P.E. Abreu, J.M.C. Marques, and F.B. Pereira *Comput. Theoret. Chem.* **975**, 83-91 (2011).

44. "Direct fit of spectroscopic data of diatomic molecules by using genetic algorithms: II. The ground state of RbCs",
M.M. Almeida, F.V. Prudente, C.E. Fellows, J.M.C. Marques, and F.B. Pereira *J. Phys. B: At. Mol. Opt. Phys.* **44**, 225102 (2011).

45. "On the use of big-bang method to generate low-energy structures of atomic clusters modeled with pair potentials of different ranges",
J.M.C. Marques, A.A.C.C. Pais, and P.E. Abreu, *J. Comput. Chem.* **33**, 442-452 (2012).

46. "Intermolecular potentials for simulations of collisions of $SiNCS^+$ and $(CH_3)_2SiNCS^+$ ions with fluorinated self-assembled monolayers",
J.J. Nogueira, A. Sánchez-Caronilla, J.M.C. Marques, W.L. Hase, E. Martínez-Núñez and S.A. Vázquez,*Chem. Phys.* **399**, 193-204 (2012).

47. "Alkali-ion microsolvation with benzene molecules",
J.M.C. Marques, J.L. Llanio-Trujillo, M. Albertí, A. Aguilar, and F. Pirani, *J. Phys. Chem. A* **116**, 4947-4956 (2012).

48. "A detailed investigation on the global minimum structures of mixed rare-gas clusters: geometry, energetics and site occupancy",
J.M.C. Marques and F.B. Pereira *J. Comput. Chem.* **34**, 505-517 (2013).

49. "Microsolvation of the potassium-ion with aromatic rings: comparison between hexafluorobenzene and benzene",
J.M.C. Marques, J.L. Llanio-Trujillo, M. Albertí, A. Aguilar and F. Pirani, *J. Phys. Chem. A* **117**, 8043-8053 (2013).

50. "New insights on lithium-cation microsolvation by solvents forming hydrogen-bonds: water versus methanol",
J.L. Llanio-Trujillo, J.M.C. Marques and F.B. Pereira, *Comput. Theoret. Chem.* **1021**, 124-134 (2013).

51. "On the lowest-energy structure of binary Zn-Cd nanoparticles: Size and composition",
C.M.A. Zanvettor and J.M.C. Marques, *Chem. Phys. Lett.* **608**, 373-379 (2014).

52. "Potassium Ion Surrounded by Aromatic Rings: Molecular Dynamics of the First Solvation Shell",
M. Albertí, A. Aguilar and J.M.C. Marques, *Eur. Phys. J. D* **68**, 364 (2014).

53. "Colloidal clusters from a global optimization perspective",
J.M.C. Marques and F.B. Pereira, *J. Mol. Liq.* **210**, 51-63 (2015).

54. "Low-energy structures of benzene clusters with a novel accurate potential surface",
M. Bartolomei, F. Pirani and J.M.C. Marques, *J. Comput. Chem.* **36**, 2291-2301 (2015).

55. "A Detailed Study on the Low-Energy Structures of Charged Colloidal-Clusters",
S.M.A. Cruz and J.M.C. Marques, *J. Phys. Chem. B* **120**, 3455-3466 (2016).

56. "Improved evolutionary algorithm for the global optimization of clusters with competing attractive and repulsive interactions", S.M.A. Cruz, J.M.C. Marques and F.B. Pereira, *J. Chem. Phys.* **145**, 154109 (2016).

57. "A global optimization perspective on molecular clusters", J.M.C. Marques, F.B. Pereira, J.L. Llanio-Trujillo, P.E. Abreu, M. Albertí, A. Aguilar, F. Pirani and M. Bartolomei, *Phil. Trans. R. Soc. A* **375**, issue: 2092, 20160198 (2017).

58. "Low-energy structures of clusters modeled with competing repulsive and either long- or moderate short-range attractive interactions", S.M.A. Cruz and J.M.C. Marques, *Comput. Theor. Chem.* **1107**, 82-93 (2017).

59. "GAFit: a general-purpose, user-friendly program for fitting potential energy surfaces", R. Rodríguez-Fernández, F.B. Pereira, J.M.C. Marques, E. Martínez-Núñez and S.A. Vázquez, *Comput. Phys. Commun.* **217**, 89-98 (2017).

60. "Modeling coronene nanostructures: analytical potential, stable configurations and ab initio energies", M. Bartolomei, F. Pirani and J.M.C. Marques, *J. Phys. Chem. C* **121**, 14330-14338 (2017).

61. "Solvation of Li^+ by argon: How important are three-body forces?", F.V. Prudente, J.M.C. Marques and F.B. Pereira, *Phys. Chem. Chem. Phys.* 19, 25707-25716 (2017).

62. "Correction: Solvation of Li^+ by argon: how important are three-body forces?", F.V. Prudente, J.M.C. Marques and F.B. Pereira, *Phys. Chem. Chem. Phys.* 20, 16877-16882 (2018).

63. "Toward the Understanding of Micro-TLC Behavior of Various Dyes on Silica and Cellulose Stationary Phases Using A Data Mining Approach", J. C. Pereira, J.M.C. Marques, E. Wlodarczyk, B. Fenert, and P.K. Zarzycki, *J. AOAC Int.* 101, 1437-1447 (2018).

64. "Two-dimensional clusters from self-assembly of oppositely charged particles", S.G. Rodrigues, A.A.C.C. Pais, and J.M.C. Marques, *Chem. Phys. Lett.* 706, 586-593 (2018).

65. "Aggregation of Cyclodextrins: Fundamental Issues and Applications", T.F.G.G. Cova, S.M.A. Cruz, A.J.M. Valente, P.E. Abreu, J.M.C. Marques, and A.A.C.C. Pais, in *Cyclodextrin: A Versatile Ingredient*, Poonam Arora and Neelima Dhingra(eds.), IntechOpen, pp 45-66 (2018).

66. "Revealing Energy Landscapes of Atomic Clusters by Applying Adaptive Bio-Inspired Algorithms", J.M.C. Marques, W.S. Jesus, F.V. Prudente, F.B. Pereira, and N. Lourenço, in *Physical Chemistry for Chemists and Chemical Engineers Multidisciplinary Research Perspectives*, A. V. Vakhrushev, R. Haghi, and J. V. de Julián-Ortiz (eds.), Innovations in Physical Chemistry: Monograph Series, Apple Academic Press, New York, chapter 3, pp 47-74 (2018).

67. "Exploring the first-shell and second-shell structures arising in the microsolvation of Li^+ by rare gases", W.S. Jesus, J.M.C. Marques, F.V. Prudente, and F.B. Pereira, *Int. J. Quantum Chem.* 119, e25860 (2019); chosen as cover article of issue 13.

68. "Molecular dynamics insights for screening the ability of polymers to remove pesticides from water", F.G.A. Estrada, J.M.C. Marques, and A.J.M. Valente, *ChemistryOpen* 8, 438-446 (2019).

69. "Microsolvation of Li^+ in a Mixture of Argon and Krypton: Unveiling the Most Stable Structures of the Clusters", W.S. Jesus, F.V. Prudente, and J.M.C. Marques, *J. Phys. Chem. A* 123, 2867-2873 (2019).

70. "Aggregation enhancement of coronene molecules by seeding with alkali-metal ions", M. Bartolomei, F. Pirani and J.M.C. Marques, *Phys. Chem. Chem. Phys.* **21**, 16005-16016 (2019).

Communications

1. "Low-energy dynamics of the $O(^3P) + OH(^2\Pi)$ reaction: dependence on the rotational quantum number of OH", A.J.C. Varandas and J.M.C. Marques
poster in 12^o *Encontro da Sociedade Portuguesa de Química* (Coimbra, Portugal, 1991).

2. "Low-energy dynamics of the $O(^3P) + OH(^2\Pi)$ reaction: dependence on the OH rotational quantum number and assessment of the nonstatistical recrossing", J.M.C. Marques and A.J.C. Varandas
poster in 13^o *Encontro da Sociedade Portuguesa de Química* (Lisboa, Portugal, 1992).

3. "Low-energy dynamics of the O + OD reaction: cross sections, nonstatistical recrossing and thermal rate coefficients", J.M.C. Marques and A.J.C. Varandas
poster in *I South European Conference on Atomic and Molecular Physics*, (Gandía, Spain, 1992).

4. "A simple method for correcting the zero-point energy problem of classical molecular dynamics", A.J.C. Varandas and J.M.C. Marques
poster in *Workshop on "Vibronic Processes in Gas Phase and Surface Scattering", in honour of Prof. Joop Los*, (Palmela, Portugal, 1993).

5. "Isotopic effect in $O + OH(D)$ reactive collisions at low energies: a theoretical study", J.M.C. Marques and A.J.C. Varandas
poster in *NATO ASI "Low Temperature Chemistry of the Atmosphere"*, (Maratea, Italy, 1993).

6. "Dynamics calculations of deuterium isotope effect in the $O + OH$ reaction", J.M.C. Marques, W. Wang and A.J.C. Varandas
poster in *Tenth European Conference on Dynamics of Molecular Collisions*, (Salamanca, Spain, 1994).

7. "Theoretical study of the reaction $H+Ar\cdots O_2 \rightarrow Ar+HO_2$", J.M.C. Marques, W. Wang, A.A.C.C. Pais and A.J.C. Varandas
poster in 2^o *Encontro Nacional de Química-Física*, (Porto, Portugal, 1995).

8. "A detailed theoretical study of the HO_2 complex formation in the $H + ArO_2$ reaction", W. Wang, J.M.C. Marques, A.A.C.C. Pais and A.J.C. Varandas
poster in *XV Encontro Nacional da Sociedade Portuguesa de Química*, (Porto, Portugal, 1996).

9. "Dynamics study of the $H + ArO_2$ reaction over a wide range of translational energies", J.M.C. Marques, W. Wang, A.A.C.C. Pais and A.J.C. Varandas
poster in *14th International Symposium on Gas Kinetics*, (Leeds, U.K., 1996).

10. "Theoretical study of the $H/O + ArO_2$ reactions", W. Wang, J.M.C. Marques, A.A.C.C. Pais and A.J.C. Varandas
poster in *III South European Conference on Atomic and Molecular Physics*, (Kos, Greece, 1996).

11. "Unimolecular dissociation of HO_2: a classical trajectory study", J.M.C. Marques and A.J.C. Varandas
oral communication in *Coimbra HCM meeting on Multichannel Reactions and Kinetic Modelling of Combustion Processes*, (Coimbra, Portugal, 1997).

12. "Rotational effects and mode specificity in dissociation of energized HO_2 molecules", J.M.C. Marques and A.J.C. Varandas
poster in *Second European Conference on Computational Chemistry*, (Lisboa, Portugal, 1997).

13. "Trajectory surface hopping calculations of the $Na + Li_2\,(X^1\Sigma_g^+)$ dissociation reaction", J.M.C. Marques, A.I. Voronin and A.J.C. Varandas
poster in *III Iberian Joint Meeting on Atomic and Molecular Physics*, (Mira, Portugal, 1998).

14. "Dynamics of the $Li + Li_2 (X^1\Sigma_g^+)$ dissociation reaction: a trajectory surface hopping study", J.M.C. Marques, A.I. Voronin and A.J.C. Varandas
poster in *VI European Conference on Atomic and Molecular Physics*, (Siena, Italy, 1998).

15. "QCT study of the HO_2 unimolecular dissociation. The Mu isotope substitution", J.L. Llanio-Trujillo, J.M.C. Marques and A.J.C. Varandas
oral communication in *Summer School on Molecular Reaction Dynamics and Chemical Kinetics*, (Copenhagen, Denmark, 2001).

16. "Trajectory surface hopping and self consistent potential calculations for $Li + Li_2$ dissociation reaction", J.M.C. Marques, A.I. Voronin and A.J.C. Varandas
oral communication in *V Encontro Nacional de Química-Física*, (Faro, Portugal, 2001).

17. "Time-dependent wave packet study of the electronically non-adiabatic dynamics: a one-dimensional model for the $Cl + H_2$ reaction", J.M.C. Marques, A. Riganelli and F.V. Prudente
poster in *International Workshop on Quantum Dynamical Concepts: From Diatomics to Biomolecules*, (Dresden, Germany, 2002).

18. "VTST and classical trajectory calculations for the $Cl + C_2H_6$ abstraction reaction. Comparison between theory and experiment", A. Fernández-Ramos, E. Martínez-Núñez, J.M.C. Marques and S.A. Vázquez
poster in *Conference on Electronic Structure: Principles and Applications*, (Sevilla, Spain, 2002).

19. "Trajectory dynamics study of the $Ar + CH_4$ collision induced dissociation: rate constant and energy transfer", J.M.C. Marques, E. Martínez-Núñez, A. Fernández-Ramos and S.A. Vázquez
poster in *XIX Encontro Nacional da Sociedade Portuguesa de Química*, (Coimbra, Portugal, 2004).

20. "Dynamics study of $ClO + O_2$ collisions and their role in the chemistry of stratospheric ozone", O.B.M. Teixeira, J.M.C. Marques and A.J.C. Varandas
poster in *XIX Encontro Nacional da Sociedade Portuguesa de Quí mica*, (Coimbra, Portugal, 2004).

21. "Modelling the O+OClO reaction: potential energy surface and thermal rate constants", J.M.C. Marques, O.B.M. Teixeira and A.J.C. Varandas
oral communication in *XXX Congresso Internacional de Químicos Teóricos de Expressão Latina (QUITEL)*, (Porto, Portugal, 2004).

22. "Theoretical study of the O + OClO reaction using an improved potential energy surface", O.B.M. Teixeira, J.M.C. Marques and A.J.C. Varandas
poster in *VII Encontro Nacional de Química-Física*, (Porto, Portugal, 2005).

23. "Influence of the potential energy function on the global minima of argon clusters", J.M.C. Marques, F.B. Pereira and T. Leitão
poster in *Intermolecular Forces and Clusters: A Symposium in Honour of Professor Anthony Stone*, (Cambridge, England, 2006).

24. "Collision-induced dissociation of methane with rare-gas atoms at hyperthermal energies: a trajectory dynamics study", J.M.C. Marques, E. Martínez-Núñez and S.A. Vázquez
oral communication in *Electronic Structure: Principles and Applications (ESPA)*, (Santiago de Compostela, Spain, 2006).

25. "Theoretical dynamics study on the ClO_3 system: the Cl + O_3, ClO + O_2 and O+OClO atmospheric reactions", J.M.C. Marques, O.B.M. Teixeira and A.J.C. Varandas
poster in *XVI European Conference on Dynamics of Molecular Systems (MOLEC)*, (Trento, Italy, 2006).

26. "Application of genetic algorithms in chemistry: from fitting the potential energy to the study of clusters", J.M.C. Marques and F.B. Pereira
poster in *XXI Encontro Nacional da Sociedade Portuguesa de Química*, (Porto, Portugal, 2008).

27. "Ferramenta *web* para o cálculo de estados vibracionais em tempo real", J.P.M. Poiares, S.P.J. Rodrigues, and J.M.C. Marques
poster in *XXI Encontro Nacional da Sociedade Portuguesa de Química*, (Porto, Portugal, 2008).

28. "A Hybrid Evolutionary Algorithm for Cluster Geometry Optimization: the importance of structural elitism", F.B. Pereira and J.M.C. Marques
poster in *Eighth International Conference on Hybrid Intelligent Systems (HIS 2008)*, (Barcelona, Spain, 2008).

29. "Generating low-energy structures of clusters with evolutionary algorithms and electronic-structure calculations", J.M.C. Marques, J.L. Llanio-Trujillo, and F.B. Pereira
poster in *Electronic Structure: Principles and Applications (ESPA)*, (Oviedo, Spain, 2010).

30. "Global geometry optimization of molecular clusters: the microsolvation of Ca^{2+} with methanol", J.M.C. Marques, J.L. Llanio-Trujillo, and F.B. Pereira
poster in *10th European Conference on Atomic and Molecular Physics (ECAMP)*, (Salamanca, Spain, 2010).

31. "Generation of Low-energy Structures of Atomic and Molecular Clusters", J.M.C. Marques and F.B. Pereira
oral presentation and **poster** in *10th European Conference on Atomic and Molecular Physics (ECAMP)*, (Salamanca, Spain, 2010).

32. "Microsolvation with argon atoms by using ab initio and DFT methods", P.E. Abreu and J.M.C. Marques
oral presentation in *11th Iberian Joint Meeting on Atomic and Molecular Physics (IBER2011)*, (Coimbra, Portugal, 2011).

33. "SAICS: Superimposing algorithm for the identification of chiral structures", J.M.C. Marques, J.L. Llanio-Trujillo, P.E. Abreu, and F.B. Pereira
poster in *11th Iberian Joint Meeting on Atomic and Molecular Physics*, (Coimbra, Portugal, 2011).

34. "Energy landscapes of atomic and molecular clusters: global optimization with evolutionary algorithms", J.M.C. Marques and F.B. Pereira
oral communication in *XXII Encontro Nacional da Sociedade Portuguesa de Química*, (Braga, Portugal, 2011).

35. "Discovering low-energy structures of atomic and molecular clusters", J.M.C. Marques
poster in *The Fifth International Symposium "Atomic Cluster Collisions" (ISACC)*, (Berlin, Germany, 2011).

36. "Superimposing algorithm for the identification of chiral structures (SAICS): application to clusters", J.M.C. Marques, J.L. Llanio-Trujillo, P.E. Abreu, and F.B. Pereira
poster in *The Fifth International Symposium "Atomic Cluster Collisions" (ISACC)*, (Berlin, Germany, 2011).

37. "State of the art methods to discover low-energy chemical structures: from atomic clusters to microsolvation", J.M.C. Marques
poster in *Electronic Structure: Principles and Applications (ESPA)*, (Barcelona, Spain, 2012).

38. "Microsolvation of alkali ions with polar and non-polar molecules", J.M.C. Marques
poster in *XI Encontro Nacional de Química-Física*, (Porto, Portugal, 2013).

39. "Monte Carlo simulation of Ni and Ag clusters: structure and thermodynamics", E.S. Monteiro and J.M.C. Marques
poster in *XI Encontro Nacional de Química-Física*, (Porto, Portugal, 2013).

40. "Microsolvation of alkali-metal ions: what do we learn from cluster structure optimization?", J.M.C. Marques
oral presentation in *XXIII Encontro Nacional da Sociedade Portuguesa de Química*, (Aveiro, Portugal, 2013).

41. "Structural and thermodynamic properties of metal clusters from Monte Carlo simulations", E.S. Monteiro and J.M.C. Marques
poster in *XXIII Encontro Nacional da Sociedade Portuguesa de Química*, (Aveiro, Portugal, 2013).

42. "Modeling colloidal clusters with short-ranged Morse potentials: energetics and structure", R.D. Oliveira and J.M.C. Marques
poster in *XXIII Encontro Nacional da Sociedade Portuguesa de Química*, (Aveiro, Portugal, 2013).

43. "Global optimization study of bimetallic clusters: geometry, energetics and site occupancy", C.M.A. Zanvettor and J.M.C. Marques
poster in *XXIII Encontro Nacional da Sociedade Portuguesa de Química*, (Aveiro, Portugal, 2013).

44. "Microsolvation of alkali-metal ions with aromatic rings", J.M.C. Marques
oral presentation in *The 7th International Conference on Theory of Atomic & Molecular Clusters (TAMC VII)*, (Birmingham, England, 2013).

45. "Structure of colloidal clusters from searching with global optimization methods", J.M.C. Marques and R.D. Oliveira
poster in *20th International Symposium on Surfactants in Solution (SIS 2014)*, (Coimbra, Portugal, 2014).

46. "Microsolvation aggregates of alkali-metal ions with aromatic rings", J.M.C. Marques
oral presentation in *5th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC2014)*, (Salamanca, Spain, 2014).

47. "Atomic clusters from a global optimization perspective", J.M.C. Marques
oral presentation in *Computational Approaches for Materials Design (CAMD)*, (Aveiro, Portugal, 2015).

48. "Global minimum structures of NaK alloy clusters by employing an evolutionary algorithm", V.R.G. Cacho and J.M.C. Marques
poster in *XXIV Encontro Nacional da Sociedade Portuguesa de Química*, (Coimbra, Portugal, 2015).

49. "Global geometry optimization with evolutionary algorithms: application to atomic, molecular and colloidal clusters", J.M.C. Marques
poster in *XXIV Encontro Nacional da Sociedade Portuguesa de Química*, (Coimbra, Portugal, 2015).

50. "Atomic and molecular clusters: discovering low-energy structures with evolutionary algorithms", J.M.C. Marques, presented in a *seminar at Faculdade Ciências da Universidade de Lisboa*, (Lisbon, Portugal, 2015).

51. "Evolutionary Algorithms for Global Geometry Optimizations: Application to Atomic and Molecular Clusters", J.M.C. Marques
oral presentation in *Algorithm Development and High-Performance Computing in Chemistry and Physics, COST MOLIM WG3 Meeting*, (Bratislava, Slovakia, 2016).

52. "Structure and dynamics of molecular clusters: a global optimization perspective", J.M.C. Marques
oral presentation in *Theoretical and Computational Studies of Non-Equilibrium and Non-Statistical Dynamics in Gas-Phase, Condensed-Phase, and Interfacial Reactions, CECAM Workshop*, (Paris, France, 2016).

53. "Solving Difficult Optimization Problems in Chemistry with Evolutionary Algorithms", J.M.C. Marques
poster in *XII Encontro Nacional de Química Física and I Encontro de Química Computacional*, (Évora, Portugal, 2016).

54. "Global Optimization with Evolutionary Algorithms: from Atomic Clusters to Charged Colloids", J.M.C. Marques
oral presentation in *Structure prediction of nanoclusters from global optimization techniques: computational strategies and connection to experiments, CECAM Workshop*, (Pau, France, 2016).

55. "Revealing the low-energy landscape of clusters: from the solvation of ions to the self-assembling of colloidal particles", J.M.C. Marques
oral presentation in *"Molecular Physics at the Edge" Symposium of the XXXVI Biennial Meeting of the Real Sociedad Española de Física*, (Santiago de Compostela, Spain, 2017).

56. "On the intimate relationship between intermolecular interactions and structure in clusters", J.M.C. Marques
oral presentation in *MOLIM Workshop on Intermolecular Interactions*, (Santiago de Compostela, Spain, 2017).

57. "On the effectiveness of DFT approaches for assessing the structure and energetics of Li^+Kr_n clusters", W.S. Jesus, J.M.C. Marques, F.V. Prudente and F.B. Pereira
poster in *MOLIM Workshop on Intermolecular Interactions*, (Santiago de Compostela, Spain, 2017).

58. "Acerca da relação entre o potencial intermolecular e a estrutura de agregados", J.M.C. Marques, presented in a *seminar at Instituto de Física of Universidade Federal da Bahia*, (Salvador, Brazil, 2018).

59. "Application of evolutionary algorithms to solve difficult problems in physical chemistry: geometry optimization and fitting", J.M.C. Marques
poster in *XIII Encontro Nacional de Química Física and II Encontro de Química Computacional*, (Faro, Portugal, 2018).

60. "Assessing the affinity between polymers and pesticides by molecular dynamics simulations", F.G.A. Estrada, A.J.M. Valente and J.M.C. Marques
poster in *XIII Encontro Nacional de Química Física and II Encontro de Química Computacional*, (Faro, Portugal, 2018).

61. "Discovering low-energy atomic clusters with machine learning", F.B. Pereira, N. Lourenço, W.S. Jesus, F.V. Prudente and J.M.C. Marques
oral presentation by F.B. Pereira in *53rd Annual Scientific Meeting of the European Society of Clinica Investigation "The Clocks of Metabolism and Disease"*, (Coimbra, Portugal, 2019); abstract published in the *European Journal of Clinical Investigation* 49 (Suppl. 1), 41 (S5-L6), 2019.

62. "Microsolvation by using computational methods based on artificial intelligence", J.M.C. Marques
oral presentation in *Computer Modeling and Simulation Day (CMS 2019)*, (Aveiro, Portugal, 2019).

63. "Microsolvation of ions by using state-of-the-art methods based on artificial intelligence", J.M.C. Marques
invited oral communication in *"Frontiers in Molecular Physics" Symposium of the XXXVII Biennial Meeting of the Real Sociedad Española de Física*, (Saragoza, Spain, 2019).

64. "Application of evolutionary algorithms to aid in the design of materials", J.M.C. Marques
poster in *XXVI Encontro Nacional da Sociedade Portuguesa de Química*, (Porto, Portugal, 2019).

Software development

- Traj2d: a computer code for trajectory dynamics calculations, J.M.C. Marques, A. Riganelli, and A.J.C. Varandas, 2003. Available from: http://www.qqesc.qui.uc.pt/

- Wavecalc: internet toolkit to solve the Schrödinger equation for various unidimensional potential models, J.P.M. Poiares, S.P.J. Rodrigues, and J.M.C. Marques, 2008. Available from: http://www.wavecalc.qui.uc.pt/

- SAICS: Superimposing algorithm for the identification of chiral structures, J.M.C. Marques, J.L. Llanio-Trujillo, P.E. Abreu, and F.B. Pereira, 2010 (most versions 1.2 and 1.3 in 2012). Available from: http://apps.uc.pt/mypage/faculty/qtmarque/

- EA_MOL: Evolutionary algorithm for the global minimum search of molecular clusters, J.L. Llanio-Trujillo, J.M.C. Marques, and F.B. Pereira, 2011. Available from: http://apps.uc.pt/mypage/faculty/qtmarque/en/software

- GAFit: program based on a genetic algorithm for fitting potential energy surfaces, R. Rodríguez-Fernández, F.B. Pereira, J.M.C. Marques, E. Martínez-Núñez and S.A. Vázquez, 2017.

Organization of scientific events

- "III Iberian Joint Meeting on Atomic and Molecular Physics", Mira (Portugal), May 4-7, 1998.
Organizing committee

- "XIX Encontro Nacional da Sociedade Portuguesa de Química", Coimbra (Portugal), April 15-17, 2004.
Organizing committee

- "20th International Symposium on Surfactants in Solution (SIS 2014)", Coimbra (Portugal), June 22-27, 2014.
  Organizing committee

- "5th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC2014)", Salamanca (Spain), July 8-11, 2014.
  Scientific committee

- "XXIV Encontro Nacional da Sociedade Portuguesa de Química", Coimbra (Portugal), July 1-3, 2015.
  Organizing committee

- Symposium "História da Química em torno de Vicente Seabra", Museu da Ciência, Universidade de Coimbra, Coimbra (Portugal), April 1-2, 2016.
  Organizing committee

- "XII Encontro Nacional de Química Física" and "I Simpósio de Química Computacional", Évora (Portugal), June 22-24, 2016.
  Organizing committee

- "Methods and Applications in Computational Chemistry (MACC_17)", Coimbra (Portugal), September 6, 2017.
  Organizing committee

- "Workshop 'How to protect water, soil, and plants production all together' '', Coimbra (Portugal), May 7, 2018.
  Organizing committee

- "XIII Encontro Nacional de Química Física" and "II Simpósio de Química Computacional", Faro (Portugal), June 4-6, 2018.
  Organizing committee and Scientific committee

- "Workshop 'Viruses and Nucleic Acids' ", Coimbra (Portugal), October 19, 2018.
  Organizing committee

- "Encontro sobre Estratégias Inteligentes para Química Computacional", Coimbra (Portugal), January 25, 2019.
  Organizing committee

- "XXVI Encontro Nacional da Sociedade Portuguesa de Química", Porto (Portugal), July 24-26, 2019.
  National organizing committee

Member of Scientific Communities

- Member of the "Sociedade Portuguesa de Química (SPQ)", and helped in the creation of the Computational Chemistry Group of SPQ.
- Manager team of the Computational Chemistry Group of SPQ (2014-2018).
- President of the Physical Chemistry Division of SPQ (2018-)

Member of Evaluation Panels

- Member of the FCT evaluation panel for selecting candidates to PhD and Posdoc grants from the Chemistry area (2015).

Scientific knowledge spread

- Organization of "Week of Science and Technology (Ciência Viva)", Departamento de Química, Universidade de Coimbra, November 18-22, 2013.
- "Ciência Viva no Laboratório - Scientific works for young people during the Summer holidays", Departamento de Química, Universidade de Coimbra, July 1-5, 2013.
- Maintenance of the Computational Chemistry Blog "Chimica in Silico", since July, 2013.
- Lecture for Summer University: "Química Computacional: 3 desafios para o século XXI", Department of Chemistry, July, 2014.
- "18^a Semana Cultural da Universidade de Coimbra", organization of scientifif knowledge spread activities, Department of Chemistry, March-April, 2015.
- Lecture for Summer University: "Química in silico: experiências computacionais", Department of Chemistry, July, 2015.
- Article for general public: "História da Química em torno de Vicente Seabra", Revista *Nova Ágora*, 83-84 (2016).
- Lecture for Summer University: "Química in silico e química in vitro: experiências com água", Department of Chemistry, July, 2016.
- Lecture for Summer University: "Química in silico e química in vitro", Department of Chemistry, July, 2018.

Academic management

- Member of the Scientific Committee of the Chemistry Department: 1995-2006, 2007- (through election).
- Departmental Erasmus Coordinator: 2008-2014.
- Vice-director of the Department of Chemistry: October, 2013-October, 2015.

Revision of scientific papers

Refereeing work has been carried out for the following international scientific journals:

- Journal of Physical Chemistry A: 1 paper (2010), 1 paper (2011)
- Journal of Physical Chemistry Letters: 1 paper (2013)
- Journal of Molecular Structure: 2 papers (2009), 1 paper (2010), 2 papers (2011), 2 papers (2013), 2 papers (2014), 1 paper (2015), 1 paper (2016), 2 papers (2017).
- Physical Chemistry Chemical Physics: 1 paper (2011), 2 paper (2013), 1 paper (2014), 2 papers (2015), 4 papers (2017), 3 papers (2018).
- Computational & Theoretical Chemistry: 1 paper (2013), 2 papers (2014), 1 paper (2015), 2 papers (2016), 1 paper (2017), 1 paper (2018).
- International Journal of Quantum Chemistry: 1 paper (2012)
- Nanoscale: 1 paper (2011).
- Physica Scripta: 1 paper (2008), 1 paper (2011), 1 paper (2012)
- Journal of Physics B: Atomic, Molecular & Optical Physics: 1 paper (2009), 2 papers (2010).
- International Journal of Molecular Sciences: 1 paper (2013).
- World Journal of Modeling and Simulation: 1 paper (2011).
- Canadian Journal of Chemistry: 1 paper (2012)
- Portugaliae Electrochimica Acta: 1 paper (2009)

- Chemical Physics: 1 paper (2015), 1 paper (2018)
- Applied Physics A: 1 paper (2017)
- Chemical Physics Letters: 1 paper (2015)
- Colloids and Surfaces A: 1 paper (2014)
- Computers and Structures: 1 paper (2016)
- Journal of Molecular Liquids: 1 paper (2016), 1 paper (2017), 2 papers (2018)
- Journal of Molecular Modeling: 1 paper (2014)
- Molecular Informatics: 1 paper (2017)
- RSC Advances: 1 paper (2014)
- Spectrochimica Acta: 1 paper (2017)
- Advances in Physics X: 1 paper (2018)
- Journal of Computational Chemistry: 1 paper (2018)

Academic activities

Juris

- Internship of Vera Mónica de Oliveira Batista, Universidade de Coimbra (Portugal), Thesis title: "Ajuste directo de curvas de energia potencial a dados espectroscópicos", November, 2001.
- Internship of Luís Pedro Viegas, Universidade de Coimbra (Portugal), Thesis title: " Dinâmica nuclear na proximidade de intersecções cónicas: espectro vibracional do MuHD", November??, 2002.
- Internship of Dora Márcia Ramos Silveira Taborda Brás, Universidade de Coimbra (Portugal), Thesis title: "Estudo da dinâmica do sistema $O + HO_2$", November??, 3003.

- Internship of Luís Pegado, Universidade de Coimbra (Portugal), Thesis title: "Calibração de superfícies de energia potencial utilizando informação espectroscópica: cálculos vibracionais para o NO_2 ($1^2A''$", December, 2004.

- Internship of Bruno Emanuel Oliveira Galamba, Universidade de Coimbra (Portugal), Thesis title: "Salbutamol. Estudo do espectro de infravermelho", March, 2005.

- Internship of Flávio Fortes Ramos Sousa, Universidade de Coimbra (Portugal), Thesis title: "Estudo cinético e dinâmico da reacção elementar $NH + N \rightarrow N_2 + H$", October??, 2005.

- Master of Osvaldo de Barros Mendes Teixeira, Universidade de Coimbra (Portugal), Thesis title: "Dinâmica Reaccional de Sistemas Tetratómicos em Química da Atmosfera", December, 2005.

- Master of João Pedro Martins Poiares, Universidade de Coimbra (Portugal), Thesis title: "Desenvolvimento de uma ferramenta web para o ensino de conceitos fundamentais de estrutura da matéria", September, 2006.

- Internship of Ana Catarina Gonçalves Simões, Universidade de Coimbra (Portugal), Thesis title: "Transporte de diferentes solutos através de filmes de acetato de celulose contendo acetonapirrol", October??, 2007.

- Internship of Diogo Pereira, Universidade de Coimbra (Portugal), Thesis title: "Estudo da interacção da efedrina com β-ciclodextrina por condutimetria e RMN", September, 2008.

- PhD of Jorge Miguel Gonçalves Sarraguça, Universidade de Coimbra (Portugal), Thesis title: "Modeling and Simulation of Polymers in Solution", October??, 2008.

- Internship of Carina Alexandra Dinis Forte, Universidade de Coimbra (Portugal), Thesis title: "Estudos de pré-formulação farmacêutica com um derivado do ácido acetilsalicílico: diflunisal", July, 2009.

- Master of Andreia Fernandes Jorge, Universidade de Coimbra (Portugal), Thesis title: "Controlling the charge of polyplexes: A theoretical and experimental approach", September, 2009.

- PhD thesis project of Andreia Fernandes Jorge, Universidade de Coimbra (Portugal), Title: "Controlo da carga de poliplexos", September, 2010.

- Statement on the PhD thesis of Sara Dinisa Oliveira Costa, Universidad Politécnica de Cartagena (Spain), Thesis title: "Aplicación de la Técnica de Dinámica Molecular al Estudio de Diferentes Sistemas Químicos Supramoleculares", October, 2010.

- PhD of Juan José Nogueira Pérez, Universidade de Santiago de Compostela (Spain), Thesis title: "Classical Trajectory Simulations of Collisions between Polyatomic Molecules and Self-Assembled Monolayer Surface", July, 2011.

- Master of Nídia Alexandre Duarte Moreira, Universidade de Coimbra (Portugal), Thesis title: "Estudo da reactividade de produtos da peroxidação do ácido linoleico", February, 2011.

- Master of Dulce Raquel Alves da Costa Andrade Gabriel, Universidade de Coimbra (Portugal), Thesis title: "Técnicas numéricas em tópicos regulamentares. A comercialização de medicamentos para uso veterinário", October, 2011.

- Supplementary member of the juri of the PhD thesis of Pablo G. Jambrina, Universidad de Salamanca (Spain), Thesis title: "Dynamics and Stereodynamics of Barrierless Reactions: Statistical and Dynamics Effects", September, 2011.

- Internship of Maria Teresa Antunes, Universidade de Coimbra (Portugal), Thesis title: " Interacção de ADN com a superfície de membranas celulares mediada por agentes compactantes", July, 2013.

- Supplementary member of the juri of the PhD thesis of Marta Sánchez Lozano, Universidad de Vigo (Spain), Thesis title: "Computational design of molecular tweezers and cranes with enhanced ion-π interactions", January, 2014.

- Master of Catarina Sofia Matos de Jesus, Universidade de Coimbra (Portugal), Thesis title: "Avaliação de Perfis de Degradação Química de um Produto Farmacêutico", July 2014.

- Master of Mariana Carvalhaes Gallo, Universidade de Coimbra (Portugal), Thesis title: "Obtenção de Sensores Electroquímicos e Ópticos Formados por Filmes Automontados de Nanopartículas de Ouro e Porfirina", July 2014.

- Master of Teresa Isabel Cardoso Valada, Universidade de Coimbra (Portugal), Thesis title: "Gestão de Resíduos", July 2014.

- Master of Mariana de Ayala Monteiro Mateus, Universidade de Coimbra (Portugal), Title: "Análise exploratória das potencialidades forenses do cabelo, com aplicação de técnicas de GC-MS", September 2014.
- Master of André Filipe Beirão Soares, Universidade de Coimbra (Portugal), Thesis title: "Bases de Schiff Aromáticas como Sensores Óticos em Solução e em Sólidos Mesoporosos", September 2014.
- Master of Damien da Costa Gonçalves, Universidade de Coimbra (Portugal), Thesis title: "Polímeros Termossensíveis", September 2014.
- Master of Luís Manuel Pires Veríssimo, Universidade de Coimbra (Portugal), Thesis title: "Propriedades de Transporte em Farmacologia Anti-tubercolósica: Estudo do Di-hidrocloreto de Etambutol", September 2014.
- Master of Rui Filipe Gonçalves Apostolo, Universidade de Coimbra (Portugal), Thesis title: "Estudo Espectroscópico dos Ácidos Trifluoroacético, Tricloroacético e Tribromoacético por Espectroscopia de Infravermelho com Isolamento de Matriz", September 2014.
- Master of Susana Takato Oliveira Manaia Carapito, Universidade de Coimbra (Portugal), Thesis title: "As Moléculas da Cor: Nas Máscaras da Viagem Filosófica (1783-1792) e num Tecido Oriental (1880)", September 2014.
- Member of the juri of the PhD thesis of Roberto Rodríguez Fernández, Universidad de Santiago de Compostela (Spain), Thesis title: "GAFit: A computational tool kit for parameterizations of potential energy surfaces", October, 2014.
- Internship of Diana Carolina dos Santos Ferreira, Universidade de Coimbra (Portugal), Thesis title: "Estudos em DFT para o radical HO_3", July 2014.
- Internship of Cátia Castanheira Caratão, Universidade de Coimbra (Portugal), Thesis title: "Reactivity of Nitrosoalkenes towards Indole Derivatives: an Approach to Heterocycles with Relevance in Medicinal Chemistry", July 2015.
- Master of Vanessa Sofia Santos Ventura, Universidade de Coimbra (Portugal), Title: "Identificação de biomarcadores para esquizofrenia", September 2015.
- Master of Patrícia Alexandra Caetano Frazão, Universidade de Coimbra (Portugal), Title: "Controlo da Qualidade em Águas de Consumo: estimativa de incertezas e validação", September 2015.

- Master of Maria João de Jesus Lopes Ferreira, Universidade de Coimbra (Portugal), Title: "Contributo para Avaliação não Invasiva da Permeação de Compostos Através da Pele por Métodos de Fluorescência", September 2015.

- Master of João Pedro Freire Barraca Cardoso Santos, Universidade de Coimbra (Portugal), Title: "Modificações Conformacionais Rápidas em Soluções Aquosas de Aminoácidos e Polímeros Policarboxílicos Induzidas por Salto de pH", September 2015.

- Master of Joana Daniela Ramos Costa, Universidade de Coimbra (Portugal), Title: "Desenvolvimento e Validação de Métodos Analíticos para Novas Formulações Farmacêuticas", September 2015.

- Master of Cristiana Filipa de Almeida Marques, Universidade de Coimbra (Portugal), Title: "Células solares sensibilizadas por corantes azo: eficiência e fotodegradação", September 2015.

- Master of Elisabete Priscila Pinto Ferreira, Universidade de Coimbra (Portugal), Title: "Identification and Characterization of Small Molecule Interactions With Transthyretin Amyloid Fibers", September 2015.

- Master of Ana Isabel Gomes Mata, Universidade de Coimbra (Portugal), Title: "Desenvolvimento de vacinas antitumorais geradas por PDT e a sua aplicação na potenciação da PDT sistémica", September 2015.

- PhD thesis project of Tânia Firmino Guerra Guerreiro Cova, Universidade de Coimbra (Portugal), Title: "Simulation of Supramolecular Systems: From Inclusion Complexes to Zipper-like Gels for Drug Delivery", September 2015.

- Master of Nélia Cristina Tadeu Tavares, Universidade de Coimbra (Portugal), Title: "Tiazolidinas: Da Catálise Enantiosseletiva à Dinâmica Molecular", September 2016.

- Master of Wasina Ribeiro dos Santos Fins, Universidade de Coimbra (Portugal), Title: "Estudo Computacional da Estrutura e Energética de Modelos Simples de Proteínas", September 2016.

- Internship of Filipe Guilherme de Almeida Estrada, Universidade de Coimbra (Portugal), Thesis title: "Estudos de dinâmica molecular da inclusão de tacrine, velnacrine e suronacrine, fármacos anti-Alzheimer, numa β-ciclodextrina", July 2017.

- PhD thesis project of Wasina Ribeiro dos Santos Fins, Universidade de Coimbra (Portugal), Title: "Modelação Computacional e Dinâmica de Motivos Estruturais em Proteínas Associadas a Síndrome de X-Frágil", September 2017.

- Master of José Manuel Santos Pereira, Universidade de Aveiro (Portugal), Title: "Computational optimization of bio-adsorbents for the removal of pharmaceuticals from water", October 2017.

- Internship of Diana da Costa Dias, Universidade de Coimbra (Portugal), Thesis title: "Coeficientes de difusão mútua do pesticida glufosinato de amónio em soluções aquosas", June 2018.

- Internship of Miroslava Kovach, Universidade de Coimbra (Portugal), Thesis title: "Interação entre polieletrólitos e superfícies com o mesmo tipo de carga mediada por polieletrólitos de carga oposta", July 2018.

- Member of the juri of the PhD thesis of Tânia Firmino Guerra Guerreiro Cova, Universidade de Coimbra (Portugal), Thesis title: "Simulation of supramolecular systems for drug delivery based on inclusion complexes", November, 2018.

Erasmus missions

- Master classes at the University of Santiago de Compostela (Spain), 2 days, 2008.

- PhD seminars at the University of Santiago de Compostela (Spain), May 11-12, 2015.

Classes

1991: As Monitor in the Chemistry Department of the University of Coimbra he has collaborated in the practical classes of a discipline that includes numerical methods and algorithms in Fortran 77.
1995: Becomes Assistant Lecturer in the Chemistry Department of the Coimbra University, and collaborates in practical classes of "Computational Chemistry" and "General Chemistry".
1995/96: Collaborates in the practical classes of "Computational Chemistry", "Inorganic Chemistry" and "General Chemistry Laboratory".
1996/97: Colaborates in theoretical and practical classes of "Computational Chemistry", and in the practical classes of "Inorganic Chemistry" and "General Chemistry Laboratory".

1997/98: Responsible for the theoretical classes of "Computational Chemistry" and "Statistical Mechanics", collaborates in the theoretical and practical classes of "Inorganic Chemistry", and in the practical classes of "General Chemistry Laboratory".
1998/99: Responsible for the theoretical classes of "Computational Chemistry", and collaborates in the practical classes of "General Chemistry Laboratory".
1999/2000: Responsible for the classes of "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation".
2000/2001: Responsible for the classes of "Computational Chemistry", "Statistical Mechanics", and "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation", and is the chemist scientific supervisor of three students doing their teaching probation work at Escola Secundária Emí dio Navarro (Viseu).
2001/2002: Responsible for the classes of "Computational Chemistry", "Molecular Modeling", and "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation", and is the chemist scientific supervisor of three students doing their teaching probation work at Escola Secundária Emí dio Navarro (Viseu).
2002/2003: Responsible for the classes of "Computational Chemistry", "Molecular Modeling", and "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation", and is the chemist scientific supervisor of three students doing their teaching probation work at Escola Secundária Emí dio Navarro (Viseu).
2003/2004: Responsible for the classes of "Computational Chemistry", "Molecular Modeling", and "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation".
2004/2005: Responsible for the classes of "Molecular Modeling", and "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation". Collaborates in the classes of "Laboratory of Chemistry Ia: general chemistry", "Laboratory of Chemistry IIb: analytical chemistry", and is the chemist scientific supervisor of two students doing their teaching probation work at Escola Integrada Gualdim Pais (Pombal).
2005/2006: Responsible for the classes of "Molecular Modeling", and "Laborotory of Quantum Chemistry, Spectroscopy, and Computational Simulation". Collaborates in the classes of "Laboratories of Chemistry Ia and Ib: general chemistry".
2006/2007: Sabbatical
2007/2008: Responsible for the classes of "Computational Chemistry" and "General Informatics". Collaborates in the classes of "Inorganic Chemistry", "Laboratories of Chemistry II: physical chemistry and analytical chemistry", "Tutorial in Chemistry", and is the chemist scientific supervisor of two students doing their teaching probation work at Escola Secundária Emí dio Navarro (Viseu).
2008/2009 Responsible for the classes of "Laboratory of Chemistry I: Chemical

Physics" and "General Informatics". Collaborates in the classes of "General Chemistry" (for biochemistry) and "Tutorial in Chemistry".
Erasmus Coordinator at the Chemistry Department.
2009/2010 Responsible for the classes of "Laboratory of Chemistry I: Chemical Physics". Collaborates in the classes of "General Chemistry" (for biochemistry), "General Informatics" and "Tutorial in Chemistry".
Erasmus Coordinator at the Chemistry Department.
2010/2011 Responsible for the classes of "Laboratory of Chemistry I: Chemical Physics", "Molecular Simulation and Modeling" (Master in Chemistry) and "General Informatics". Collaborates in the classes of "Tutorial in Chemistry".
Erasmus Coordinator at the Chemistry Department.
2011/2012 Responsible for the classes of "Laboratory of Chemistry I: Chemical Physics", "Physical Chemistry I" and "General Informatics". Collaborates in the classes of "Tutorial in Chemistry" and "Communication and New Technologies in Sciences Teaching" (PhD course in Sciences Teaching).
Erasmus Coordinator at the Chemistry Department.
2012/2013 Responsible for the classes of "Laboratory of Chemistry I: Chemical Physics", "Physical Chemistry I", "Molecular Simulation and Modeling" (Master in Chemistry) and "General Informatics". Collaborates in the classes of "Communication and New Technologies in Sciences Teaching" (PhD course in Sciences Teaching).
Erasmus Coordinator at the Chemistry Department.
2013/2014 Responsible for the classes of "Laboratory of Chemistry I: Chemical Physics", "Molecular Simulation and Modeling" (Master in Chemistry) and "General Informatics". Collaborates in the classes of "Molecular Modeling" (Master in Medicinal Chemistry), "Physical Chemistry I" and "Chemoinformatics".
Erasmus Coordinator at the Chemistry Department.
2014/2015 Responsible for the classes of "Physical Chemistry I", "Molecular Simulation and Modeling" (Master in Chemistry) and "General Informatics". Collaborates in the classes of "Molecular Modeling" (Master in Medicinal Chemistry) and "Chemoinformatics".
2015/2016 Responsible for the classes of "Molecular Simulation and Modeling" (Master in Chemistry) and "General Informatics". Collaborates in the classes of "Inorganic Chemistry", "Physical Chemistry I", "Molecular Modeling" (Master in Medicinal Chemistry) and "Chemoinformatics".
2016/2017 Responsible for the classes of "Molecular Simulation and Modeling" (Master in Chemistry), "General Informatics" and "Physical Chemistry I". Collaborates in the classes of "Inorganic Chemistry", "Molecular Modeling" (Master in Medicinal Chemistry) and "Chemoinformatics".
2017/2018 Responsible for the classes of "Molecular Simulation and Modeling"

(Master in Chemistry), "General Informatics" and "Physical Chemistry I". Collaborates in the classes of "General Chemistry I", "Inorganic Chemistry", "Molecular Modeling" (Master in Medicinal Chemistry) and "Chemoinformatics".
2018/2019 Responsible for the classes of "Molecular Simulation and Modeling" (Master in Chemistry), "General Informatics" and "Physical Chemistry I". Collaborates in the classes of "General Chemistry I", "Molecular Modeling" (Master in Medicinal Chemistry) and "Chemoinformatics".