Sarantos Marinakis

EDUCATION

2013 – 2015 Post-Graduate Certificate in Academic Practice (PGCAP), Queen Mary U. of London, UK 2001 – 2006 D. Phil., University of Oxford, UK

'The Dynamics of Inelastic and Reactive Bimolecular Collisions'. Supervised by Prof. M. Brouard. Work involved laser-induced fluorescence experiments and quantum beat spectroscopy. I also took the initiative to study inelastic collisions of nitric oxide, through which I fostered productive collaborations between groups in Oxford, Madrid, and Prof. Stolte's group at Amsterdam resulting in 2 publications. When Prof. Stolte stopped experiments, he donated the apparatus to Oxford. Thus my initiative brought equipment worth around £1m to Oxford and provided a good home to an experiment that might have otherwise disappeared.

1997 – 1999 M. Sc., University of Athens, Greece

'Computer Simulation Study of the Xe/N₂ Mixture in the Supercritical Region'. Supervised by Prof. I. Samios

1992 – 1997 First Degree in Chemistry, University of Athens, Greece

PROFESSIONAL EXPERIENCE

Sep 2020 - Present Associate Professor in Physical Chemistry and Spectroscopy, U. of Patras, GR

Jul 2019 - Sep 2020 Senior Lecturer in Inorganic and Physical Chemistry, U. of East London, UK

Aug 2018 - June 2019 Lecturer in Inorganic and Physical Chemistry, U. of East London, UK

Sep 2015 - July 2018 Lecturer in Inorganic and Physical Chemistry, Queen Mary U. of London, UK

Aug 2013 - Aug 2015 Lecturer in Physical Chemistry, Queen Mary U. of London, UK

Nov 2009 – Apr 2013 Postdoctoral researcher, University of Oxford, UK

Dec 2008 – **Nov 2009** Postdoctoral researcher, Université Pierre-et-Marie-Curie (Paris 6), France Worked with Prof. M.-L. Dubernet on *ab initio* calculations of potential energy surfaces and was responsible for the scientific content of BASECOL, a useful astronomical database.

Dec 2008 - Nov 2009 Academic Visitor, University of Oxford, UK (non-stipendiary)

Nov 2005 – Nov 2008 Research Associate, Heriot-Watt University, UK

In Prof. McKendrick's group, I built a challenging experimental apparatus for polarisation spectroscopy with a total budget of around £500k. I also performed quantum mechanical calculations in collaboration with Dr Kłos (Maryland, USA). The group became a world leader in elastic depolarizing collisions and members were invited to present the results of our work in highly respected journals and at all the highly-rated conferences in my field.

Mar 2002 – Mar 2004 Pre-doctoral researcher in an EU Research Training Network

Nov 1999 – May 2001 Military Service (required by Greek law)

TEACHING EXPERIENCE

Mar 2023 – Present Lecturer in Atmospheric Chemistry for the post-graduate course Environmental Sciences, U. of Patras, GR

Sep 2020 - Present Associate Professor in Physical Chemistry and Spectroscopy, U. of Patras, GR

Jul 2019 - Present Senior Lecturer in Inorganic and Physical Chemistry, U. of East London, UK

Aug 2018 – June 2019 Lecturer in Inorganic and Physical Chemistry, U. of East London, UK

Sep 2015 – Jul 2018 Lecturer in Inorganic and Physical Chemistry, Queen Mary U. of London, UK

Sep 2014 Member in the MSc Exam Board at Queen Mary University of London, UK

Aug 2013 - Aug 2015 Lecturer in Physical Chemistry, SBCS, Queen Mary University of London, UK

Sep 2011 – Dec 2012 Tutor of Quantum Chemistry Supplementary Course to undergraduate students, University of Oxford, UK

Sep 2010 – June 2011 Junior Demonstrator of Physical Chemistry experiments to undergraduate students, University of Oxford, UK

Jan 2010 – June 2010 College Tutor for Pembroke College, teaching physical chemistry to undergraduate students, University of Oxford, UK

Jan 2006 - Nov 2008 Tutor of 'Mathematics for Chemists', 'Quantum Mechanics and Spectroscopy',

'Statistical Mechanics', and demonstrated experiments to undergraduate students, Heriot-Watt University, UK. Awarded Approved Tutor status after completing teaching training LEADS 1,2.

Oct 2004 – Jun 2005 College tutor for Keble and St. Hugh's Colleges, teaching Mathematics to undergraduate students, University of Oxford, UK

Sep 1998 – Sep 1999 Teaching assistant at the University of Athens, Greece

OTHER PROFESSIONAL EXPERIENCE

9/2025 Chair of the International Conference on Physical Chemistry and Spectroscopy, Patras, Greece

6/2025 Referee in Academia Quantum journal

6/2025 Referee in The Journal of Applied Physics journal

5/2025 Member in the commission for PhD defence at the Democritus University of Thrace, Greece

2/2025 Referee in New Materials, Compounds and Applications journal

1/2025 Referee in The Journal of Applied Physics journal

12/2024 Referee in The Journal of Chemical Physics journal

11/2024 Member of the Adjudication Committee for Ph. D. thesis at GITAM (Deemed to be University)

7/2024 - Present Member of the PhD Advisory Panel at Department of Chemistry, Democritus University of Thrace

6/2024 Referee for RSC Researcher Collaborations

1/2024 Referee in Computational and Theoretical Chemistry journal

9/2023 Referee for RSC Researcher Collaborations

9/2023 Chair of the International Conference on Physical Chemistry and Spectroscopy,

Patras, Greece

9/2023 - Present Referee in ChemPhysChem journal

7/2023 Referee for RSC Research Fund

5/2023 Referee for RSC Research Fund

1/2023 Referee for RSC Research Fund

11/2022 Referee for RSC Research Enablement Grant

8/2022 Referee for RSC Research Fund

5/2022 Referee for RSC Undergraduate Research Bursaries

1/2022 Referee for RSC Research Fund

11/2021 Referee for RSC Research Enablement Grant

9/2021 Chair of the International Conference on Physical Chemistry and Spectroscopy, Patras, Greece

7/2021 Referee for RSC Research Fund and Research Enablement Grant

3/2021 Referee for RSC Foundation undergraduate research bursaries

11/2020 Referee for RSC Foundation undergraduate summer research bursaries

10/2020 Referee for Marie Sklodowska-Curie Individual Fellowships

6/2020 Referee for EPSRC Peer Review Extranet

3/2020 Member in the commission for PhD defence at the University of Patras, Greece

11/2019 Referee Marie Sklodowska-Curie Individual Fellowships

7/2019 Referee for software for Oxford University Press

3/2019 Referee for RSC Foundation undergraduate summer research bursaries

3/2019 Referee for EPSRC-UK

11/2018 Appeals committee member for Proposals for HFRI (Hellenic Foundation for Research and Innovation – Greece)

11/2018 Referee Marie Sklodowska-Curie Individual Fellowships

5/2018 Reviewer for Books for Pearson Publishing

4/2018 Member of the Editorial Board for the Journal of Physical Chemistry and Functional Materials

4/2018 Referee for RSC/Nuffield Foundation undergraduate summer research bursaries

3/2018 Referee for EPSRC-UK

1/2018 Referee for Proposals for GRNET High Performance Computing Services

10/2017 Member of the PhD Advisory Panel at Queen Mary University of London

9/2017 - Present Referee in Astrophys. J. journal

1/2017 Member of the Steering Group of the Teaching and Learning Conference, Queen Mary, University of London, UK

12/2016 Referee for Proposals for GRNET High Performance Computing Services

9/2016 Member of the Engineering and Physical Sciences Research Council (EPSRC-UK) Peer Review Associate College

7/2016 Evaluator for Books Proposal for Oxford University Press

7/2016 Member of the Scientific Committee of the 6th International Meeting on

Atomic and Molecular Physics and Chemistry, Le Havre, France

1/2016 Member of the Steering Group of the Teaching and Learning Conference, Queen Mary, University of London, UK

11/2015 Member of the Subject Expert Grant Assessment Panel for RSC/Researcher Mobility Grant Applications

7/2015 – Present Evaluator for RSC/Open education resources

7/2015 - Present Referee in Mon. Not. R. Astron. Soc. journal

5/2015 Referee for RSC/Researcher mobility fellowship

5/2015 Referee for RSC/Nuffield Foundation undergraduate summer research bursaries

10/2014 - Present Referee for EPSRC-UK

9/2014 Referee for Books Proposal for Academic Press/Elsevier

9/2014 Member in the MSc Exam Board at Queen Mary University of London

6/2014 Referee for RSC/Researcher mobility fellowship

3/2014 Referee for RSC/Nuffield Foundation undergraduate summer research bursaries

3/2013 Referee for RSC/Nuffield Foundation undergraduate summer research bursaries

1/2013 Member in the commission for PhD defence at the University of Nijmegen, The Netherlands

9/2012 Undergraduate admissions interviewer for Pembroke College

9/2009 - Present Referee in Chem. Phys. Lett. journal

1/2009 Co-Chair of Gordon Research Conference: Molecular Energy Transfer, Graduate Research Seminar, California, USA

Constructed a diverse meeting with presentations on topics ranging from diatomics to biochemistry by a range of international speakers. The high participation, financial success and the positive comments from participants secured the continuation of this seminar.

12/2007 - Present Referee in Phys. Chem. Chem. Phys. journal

4/2007 Participated in the translation into Greek of engaging educational software for Chemistry in secondary schools

PROFESSIONAL MEMBERSHIPS

Fellow of the Higher Education Academy (from 2015)

Member of the American Chemical Society (from 2009)

Member of the Royal Society of Chemistry (from 2001)

Member of the Greek Society of Chemistry (from 1997)

CURRENT RESEARCH PROJECTS

I have fostered several on-going collaborations with researchers in the UK and abroad on a rich variety of projects including:

- *Ab initio* quantum mechanical calculations of van der Waals complexes (Prof. B. J. Howard, Oxford, UK; Prof. G. Groenenboom, Nijmegen, The Netherlands)
- Astrophysical chemistry (Dr I. Jiménez-Serra, London, UK; Prof. S. Viti, London, UK; Dr F. Lique, Le Havre, France)
- Cold molecules (Prof. P. Barker, London, UK)
- Experimental and theoretical studies of gas phase collisions (Dr S. Althorpe, Cambridge, UK; Prof. F.
- J. Aoiz, Madrid, Spain; Dr J. Kłos, Maryland, USA; Prof. K. G. McKendrick, Edinburgh, UK; Prof. D. Parker, Nijmegen, The Netherlands; Prof. S. Stolte, Jilin, China)
- Experimental and theoretical studies of nitric oxide complexes (Prof. M. H. Alexander and Dr J. Kłos, Maryland, USA; Prof. B. J. Howard, Oxford, UK; Dr T. Kraemer, Edinburgh; Dr T. Sheriff, London; Dr N. Walker, Newcastle, UK)
- Neutron scattering and molecular dynamics simulation of supercritical fluids (Prof. I. Samios, Athens, Greece; Dr A. Soper, Rutherford, UK)
- Studies of Indocyanine Green and Infrared Fluorescent Protein (Dr A. Bassi, Milan, Italy; Dr G. Chass, London, UK)
- Terahertz spectroscopy (BrightSpec, Virginia, USA; Dr G. Chass, London, UK)
- Inorganic Pigments in Paintings (Dr D. Peggie, National Gallery, UK)

IT

Programming in: GWBasic, COBOL, FORTRAN, MATLAB, Python, Visual C++,

Operating Systems: Windows 11, UNIX, MS-DOS, Linux

Packages: Adobe Illustrator, Corel Draw, Endnote, Excel, Gaussian, GaussView, LabVIEW, LaTeX, Maple, Mathematica, Molpro, Netscape Composer, Origin, PowerPoint, SPFIT, Surfer, Teams, Word, Zotero

GRANTS AND AWARDS

- 28. 2024 ARIS, (Greek) National High Performance Computing System; Awarded 1000000 CPU hours
- 27. 2024 ARIS, (Greek) National High Performance Computing System; Awarded 100000 CPU hours
- 26. 2024 U. of Patras, Funding for computational software; Awarded 12102 €
- 25. 2023 Erasmus+, Funding for research visit to IPR University of Rennes; Awarded 1368 €
- 24. 2023 U. of Patras, Funding for organizing the International Conference on Physical Chemistry and Spectroscopy; Awarded 1000 €
- 23. 2021 U. of Patras, Funding for organizing the International Conference on Physical Chemistry and Spectroscopy; Awarded 1000 €
- 22. 2020 UEL Internal Internship; 'Monitoring key air-pollutants in the Docklands resulting the taking off and landing of airplanes from City Airport'; Awarded £1700
- 21. 2019 Science and Technology Facilities Council (STFC); 'Watching the birth and death of chemical bonds with pulsed neutrons: The case of nitric oxide'; Awarded (Co-I)
- 20. 2019 UEL Internal Internship; 'Monitoring the air-pollution in the most affected areas in Tower Hamlets, London'; Awarded £3545
- 19. 2018 Science and Technology Facilities Council (STFC); 'Microscopic structure of nitric oxide (NO): A comparison between experiments and theory'; Notional value £43.5k
- 18. 2017 Science and Technology Facilities Council (STFC); 'Microscopic structure as an evidence for a new thermodynamic boundary in supercritical CO₂: A comparison between experiments and theory'; Notional value £114.48k
- 17. 2016 Science and Technology Facilities Council (STFC); 'Local intermolecular structure and dynamics in binary supercritical mixtures'; Notional value £127.7k
- 16. 2016 European Cooperation in Science and Technology COST, Chemistry and Molecular Sciences and Technologies (CMST) CM1401; Awarded 750 €
- 15. 2015 Centre for Public Engagement, QMUL; Awarded 200 GBP to prepare a podcast
- 14. 2015 Science without Borders; Awarded 1200 GBP to train Brazilian undergraduate student in chemistry research methods
- 13. 2014 UK National Service for Computational Chemistry Software; Awarded 95000 CPU hours
- 12. 2013 Lockey Committee travel bursary to attend a Conference
- 11. 2012 Lockey Committee travel bursary to attend a Conference
- 10. 2012 Oxford Supercomputing Centre; Awarded 25000 CPU hours
- 9. 2011 University of Athens, Greece (computational time and software for studies of biological molecules)
- 8. 2011 UK National Service for Computational Chemistry Software; Awarded 71000 CPU hours
- 7. 2011 Oxford Supercomputing Centre; Awarded 3500 CPU hours
- 6. 2010 British Council-Platform Beta Techniek Programme in Science to collaborate with Prof. Parker's group (Nijmegen, NL)
- 5. 2008 Collaborative Computational Project on Molecular Quantum Dynamics (CCP6) travel bursary to collaborate with Dr Althorpe's group (Cambridge, UK)
- 4. 2008 British Council support to develop a collaboration with Dr Bassi's group (Milan, Italy)
- 3. 2007 British Council-NWO Partnership Programme in Science (PPS 883) to collaborate with Prof. Stolte's group (Amsterdam, NL)
- 2. 2001-2005 D. Phil. scholarship for studies abroad (awarded after competitive written examinations) from the Greek State Scholarships Foundation (IKY)
- 1. 1998 Award based on performance from the Greek State Scholarships Foundation (IKY)

RESEARCH INTERESTS

Ab initio calculations of van der Waals complexes, density functional theory calculations and infrared/Raman/ultra-violet/visible spectroscopy of biologically relevant molecules (nitrosyl complexes and dyes), inelastic scattering, laser-induced fluorescence, microwave spectroscopy, molecular astrochemistry, molecular dynamics simulations, neutron scattering, polarization spectroscopy, quantummechanical scattering calculations, quasi-classical trajectory calculations, reaction dynamics, study of cocrystals, study of wines, and transport and relaxation properties of supercritical fluids

REFEREES

Prof. B. J. Howard (Supervisor in previous post-doc position), PTCL, Chemistry Department, University of Oxford, South Parks Road, OX1 3QZ, Oxford, UK brian.howard@chem.ox.ac.uk Tel. 0044 186 527 5438

Prof. K. G. McKendrick (Supervisor in previous post-doc position), EPS School, Heriot-Watt University, EH14 4AS, Edinburgh, UK k.g.mckendrick@hw.ac.uk Tel. 0044 131 451 3109

Prof. R. W. Pickersgill (Head of School of Biological and Chemical Sciences), J. P. Building, SBCS, Queen Mary University of London, Mile End Road, E1 4NS, London, UK r.w.pickersgill@qmul.ac.uk Tel. 0044 207 882 8882

SEMINARS, CONFERENCES (selected)

- 58. International Conference on Physical Chemistry and Spectroscopy, 'Interactions and clustering of free radicals in the liquid phase', Patras, Greece, September, 2025 (talk)
- 57. 17th Meeting of the Hellenic Society of Basic and Clinical Pharmacology, 'Crystal structure of a cocrystal formed by lamotrigine and citric acid agents', K. Tsiakopoulou*, **S. Marinakis**, N. Bouropoulos, P. G. Koutsoukos, V. Psycharis, Department of Pharmacy, National and Kapodistrian University of Athens (NKUA), Athens, Greece, May, 2025 (poster)
- 56. 2025 North America, Greece and Cyprus Conference (NAGC), 'Crystal structure of a cocrystal formed by lamotrigine and citric acid agents', K. Tsiakopoulou, **S. Marinakis**, N. Bouropoulos, P. G. Koutsoukos, V. Psycharis*, Syros, Greece, May, 2025 (talk)
- 55. University of Oxford, 'Studying the life and death of radicals: The case of NO', Oxford, UK, September, 2024 (talk)
- 54. University of Rennes, 'Recent progress in studying dimerization of nitrogen monoxide and selective deposition of hydroxyapatite', Rennes, France, June, 2024 (talk)
- 53. 14th National (Greek) Congress of Chemical Engineering, 'Electronic and magnetic properties of Prussian Blue obtained using periodic DFT', P. Leventis*, N. N. Lathiotakis, **S. Marinakis**, Thessaloniki, Greece, May, 2024 (poster and talk)
- 52. 14th National Congress of Chemical Engineering, 'Study of calcification of polymeric membranes with antimicrobial action', P. Maroulis*, P. D. Natsi, I. Tzoumani, **S. Marinakis**, E. Dalas, P. G. Koutsoukos, Thessaloniki, Greece, May, 2024 (poster)
- 51. International Conference on Physical Chemistry and Spectroscopy, 'Studying nitric oxide in the liquid, gas, and solid states', Patras, Greece, September, 2023 (talk)
- 50. University of Rennes, 'Studying nitric oxide in the liquid and gas phase', Rennes, France, June, 2023 (talk)
- 49. University of East London, 'Applications of the density functional theory on the study of penicillins', London, UK, April, 2022 (talk)
- 48. University of East London, 'Distribution of species in aquatic systems', London, UK, February, 2022 (talk)
- 47. National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, 'Understanding the supercritical state through experiments and calculations', Athens, Greece, October, 2021 (talk)
- 46. International Conference on Physical Chemistry and Spectroscopy, 'Experimental and modelling studies on supercritical CO₂ and Ar / Xe-N₂ mixtures', Patras, Greece, September, 2021 (talk)

- 45. University of East London Summer Research Conference, 'Research is Open', 'Astrophysical chemistry and radicals', London, UK, July, 2020 (talk)
- 44. Max Planck Institute for Radio Astronomy, 'Collisions of free radicals and astrophysical chemistry', Bonn, Germany, July, 2020 (talk)
- 43. Materials Chemistry Consortium Meeting, 'Systems containing NO and CO₂: experiments, theory and applications', UCL, London, UK, January 2020 (talk)
- 42. 39th International Conference and CCP5 Annual General Meeting, London, 'Supercritical fluids: microscopic structure and dynamics', September 2019 (talk)
- 41. Université du Havre, 'Microscopic structure, dynamics, and spectroscopy in supercritical gases: comparison between theory and experiment', Le Havre, France, May 2019 (talk)
- 40. University of Oxford, 'Recent experimental and theoretical progress in understanding the microscopic structure and dynamics in supercritical fluids: CO₂, Ar/Xe-N₂', Oxford, UK, March 2019 (talk)
- 39. Atomic and Molecular Interactions (AMIG) Summer Meeting, 'Collisions of free radicals important in astrophysical chemistry', London, UK, June 2018 (talk)
- 38. European Cooperation in Science and Technology (COST) Action CM1401, 'Rotational excitation of interstellar radicals (OH, CH, and PO) with He', Faro, Portugal, January 2017 (talk)
- 37. Joint European Molecular Liquids Group and Japanese Molecular Liquids Group Annual Meeting, 'A joint experimental and molecular dynamics study of the Xe/N₂ supercritical mixture', Chania, Greece, September 2016 (poster)
- 36. International Meeting on Atomic and Molecular Physics and Chemistry, 'An experimental and theoretical study of [NiBr(NO)(PPh₃)₂]', Le Havre, France, June 2016 (talk)
- 35. Queen Mary University of London, 'Understand feedback: delivery and use', QMUL Teaching and Learning Conference, London, UK, January 2016 (talk)
- 34. International Meeting on Atomic and Molecular Physics and Chemistry, 'Cold matter and OH radicals', Birmingham, UK, August 2015 (talk)
- 33. International Symposium on Atomic Cluster Collisions, 'Collisions of OH radicals', Madrid, Spain, July 2015 (talk)
- 32. NSCCS, 'Study of nitrosyl complexes', Imperial College London, UK, February 2015 (lightning talk and poster)
- 31. International Conference on High Resolution Molecular Spectroscopy, 'Zeeman effects in open-shell van der Waals complexes: the ArNO case', Bologna, Italy, September 2014 (poster)
- 30. Université du Havre, 'Collisions of OH and CH radicals', Le Havre, France, June 2014 (talk)
- 29. Université Joseph Fourier, 'Rotational excitation of OH and CH radicals', Grenoble, France, February 2014 (talk)
- 28. NSCCS, 'Magnetic effects in free radicals complexes probed by microwave experiments and effective Hamiltonians', Imperial College London, UK, December 2013 (poster)
- 27. Université du Havre, 'Quantum beat spectroscopy of NO(A)', Le Havre, France, May 2013 (talk)
- 26. Gordon Research Conference on Molecular Energy Transfer, 'Zeeman effects in open-shell van der Waals complexes', Ventura California, USA, January 2013 (poster)
- 25. NSCCS, 'Zeeman effects in open-shell van der Waals complexes', Imperial College London, UK, December 2012 (talk)
- 24. International Conference on High Resolution Molecular Spectroscopy, 'Zeeman effects in open-shell van der Waals complexes', Prague, Czech Republic, September 2012 (poster)
- 23. University of Oxford, 'Hyperfine structure of NO($A^2\Sigma^+$)', Oxford, UK, Hilary Term 2012 (talk)
- 22. RSC Spectroscopy and Dynamics Group, 'NO(X)-X systems: A combined microwave spectroscopy and quantum study', University of Leicester, Leicester, UK, January 2012 (poster)
- 21. International Conference on Molecular Energy Transfer, 'Product rotational alignment in NO(X) + Kr collisions', Oxford, UK, September 2011 (poster)
- 20. Radboud University, 'Recent experimental and theoretical investigation of Kr-NO', Nijmegen, The Netherlands, March 2011 (talk)
- 19. RSC Spectroscopy and Dynamics Group, 'The NO(X)-Kr complex: A combined microwave spectroscopy and quantum study', Heriot-Watt University, Edinburgh, UK, January 2011 (poster)
- 18. University of Oxford, 'Studies of NO-X complexes', Oxford, UK, March 2010 (talk)

- 17. Radboud University, 'Recent experimental and theoretical investigation of OH Δm_j collisions', Nijmegen, July 2009 (talk)
- 16. Advanced Workshop on Theoretical and Computational Methods for Molecular Spectroscopy and Collisions, 'Separating elastic and inelastic collisions: Experiment and theory', Granada, Spain, May 2009 (talk)
- 15. Gordon Research Conference on Molecular Energy Transfer, 'The BASECOL collisional excitation database', Ventura California, USA, January 2009 (poster)
- 14. Gordon Research Conference on Molecular Energy Transfer, 'Inelastic collision dynamics in open-shell systems: He + NO($X^2\Pi$)', Ventura California, USA, January 2009 (poster)
- 13. Building a successful international research career, British Council, Paris, France, February 2008 (invited to attend)
- 12. RSC Spectroscopy and Dynamics Group, 'Inelastic and elastic scattering of OH + Ar/He: experiment and theory', University of East Anglia, UK, December 2007 (talk)
- 11. Graduate Research School, 'Inelastic and elastic scattering of OH + Ar/He: theory and experiment', Arcachon, France, June 2007 (talk)
- 10. Stereodynamics of Chemical Reactions, 'Collisional and non-collisional depolarization of OH rotational angular momentum alignment', Arcachon, France, November 2006 (poster)
- 9. RSC Spectroscopy and Dynamics Group, 'Spotting rotational rainbows in inelastic scattering: The He-NO case', University of Durham, UK, December 2005 (poster)
- 8. RSC Spectroscopy and Dynamics Group, 'Collisional depolarization of OH(A) studied by Zeeman quantum beat spectroscopy', University of Leicester, UK, December 2004 (poster)
- 7. 18th International Symposium on Gas Kinetics, 'The reaction H + H₂O and H + D₂O: Stereodynamics and new values for the integral cross sections', Bristol, UK, August 2004 (poster)
- 6. Gordon Research Conference on Atomic & Molecular Interactions, 'H + H₂O abstraction reaction: Isotopic and spin-orbit effects', Colby-Sawyer College, New Hampshire, USA, July 2004 (poster)
- 5. Faraday Discussion 127, Non-Adiabatic Effects in Chemical Dynamics, 'Product spin-orbit dependence of the H + D₂O abstraction reaction dynamics', Oxford, UK, April 2004 (poster)
- 4. RSC Spectroscopy and Dynamics Group, 'Stereodynamics of the H + D₂O abstraction reaction at 2.46 eV', University of East Anglia, UK, December 2003 (poster)
- 3. Reaction Dynamics EU Network Meeting, 'The dynamics of the H + H₂O abstraction reaction', Nijmegen, The Netherlands, May 2003 (talk)
- 2. Stereodynamics of Chemical Reactions, 'The integral cross section for the H + H₂O abstraction reaction at 2.46 eV', Schoorl, The Netherlands, December 2002 (poster)
- 1. Reaction Dynamics EU Network Mid-Term Review Meeting, 'The integral cross sections for the H + H₂O abstraction reaction', Segovia, Spain, June 2002 (talk)

PUBLICATIONS (Researcher ID: C-7216-2011, ORCID: 0000-0002-9367-4527)

- 42. C. Cockrell, K. Trachenko, T. F. Headen, A. K. Soper, P. Hadjidoukas, G. Katsidima, S. Marinakis*, 'Molecular dynamics simulations of liquid nitrogen monoxide', *J. Mol. Liq.*, 437B (8pp), 128434, DOI: 10.1016/j.molliq.2025.128434
- 41. M. Zervos, I. Paschos, P. Savvidis, N. Florini, K. Koutsokostas, P. Komninou, N. L. Lathiotakis, P. M. Levendis, **S. Marinakis**, 'High crystal quality and purity Cu₂O by consecutive in-situ annealing and thermal oxidation of Cu under H₂ and O₂ at elevated temperatures', *CrystEngComm*, 27, 1977-1985 (2025), DOI: 10.1039/D4CE01276C
- 40. N. Georgopoulou, I. Necitailaite, C. D. Zeinalipour-Yazdi, D. Palles, G. Mousdis, C. Garoufalis, S. Marinakis*, 'Experimental and theoretical investigation of GS-441524 using Density Functional Theory, FTIR, Raman, and UV-VIS spectroscopy', *J. Eng. Sci. Tech.* 17(5), 1-7 (2024), DOI: 10.25103/jestr.175.01
- 39. M. L. Dubernet*, C. Boursier, O. Denis-Alpizar, Y. A. Ba, N. Moreau, C. M. Zwölf, M. A. Amor, D. Babikov, N. Balakrishnan, C. Balança, M. Ben Khalifa, A. Bergeat, C. T. Bop, L. Cabrera-González, C. Cárdenas, A. Chefai, P. J. Dagdigian, F. Dayou, S. Demes, B. Desrousseaux, F. Dumouchel, A. Faure, R. C. Forrey, J. Franz, R. M. García-Vázquez, F. Gianturco, A. Godard Palluet, L. González-Sánchez, G. C. Groenenboom, P. Halvick, K. Hammami, F. Khadri, Y. Kalugina, I. Kleiner, J. Kłos, F. Lique, J. Loreau, B. Mandal, B.

- Mant, S. Marinakis, D. Ndaw, P. Pirlot Jankowiak, T. Price, E. Quintas-Sánchez, R. Ramachandran, E. Sahnoun, C. Santander, P. C. Stancil, T. Stoecklin, J. Tennyson, F. Tonolo, R. Urzúa-Leiva, B. Yang, E. Yurtsever, and Michal Zóltowski., 'BASECOL2023 scientific content', *Astron. Astrophys.*, 683, A40 (31pp) (2024), DOI: 10.1051/0004-6361/202348233
- 38. A. Dimitropoulos, Ch. Stamou, Sp. P. Perlepes, Z. G. Lada, I. D. Petsalakis, **S. Marinakis***, 'A study of 1-methylbenzotriazole (MEBTA) using quantum mechanical calculations and vibrational, electronic, and nuclear magnetic resonance spectroscopies', *J. Eng. Sci. Tech. Rev.*, 16, 4, 77-84 (2023), DOI: 10.25103/jestr.164.10
- 37. **S. Marinakis**, C. Cockrell, K. Trachenko, T. F. Headen, A. K. Soper, 'The microscopic structure of liquid nitric oxide', *J. Phys. Chem. B*, 126, 47, 9860-9870 (2022), DOI: 10.1021/acs.jpcb.2c05384
- 36. B. Desrousseaux, E. Quintas-Sánchez, R. Dawes, **S. Marinakis**, F. Lique, 'Collisional excitation of interstellar PN by H₂: new interaction potential and scattering calculations', *J. Chem. Phys.*, 154, 034304 (9pp) (2021), DOI: 10.1063/5.0039145
- 35. C. Cockrell, O. Dicks, L. Wang, K. Trachenko, A. Soper, V. V. Brazhkin, **S. Marinakis***, 'Experimental and modelling evidence for structural crossover in supercritical CO₂', *Phys. Rev. E*, 101, 052109(6pp) (2020) DOI: 10.1103/PhysRevE.101.052109
- 34. V. M. Rivilla*, M. N. Drozdovskaya, K. Altwegg, P. Caselli, M. T. Beltrán, F. Fontani, F. F. S. van der Tak, R. Cesaroni, A. Vasyunin, M. Rubin, F. Lique, **S. Marinakis**, L. Testi, and the ROSINA team, 'ALMA and ROSINA detections of phosphorus-bearing molecules: the interstellar thread between star-forming regions and comets', *Mon. Notices Royal Astron. Soc.*, 492, 1180-98 (2020), DOI: 10.1093/mnras/stz3336 (mentioned in ESO/INAF press release: https://www.hq.eso.org/public/news/eso2001)
- 33. **S. Marinakis***, Y. Kalugina, J. Kłos, F. Lique, 'Hyperfine excitation of CH and OH radicals by He', *Astron. Astrophys.*, 629, A130(5pp) (2019) DOI: 10.1051/0004-6361/201936170
- 32. A. Soper, I. Skarmoutsos, J. Kłos, I. Samios, **S. Marinakis***, 'A study of Ar-N₂ supercritical mixtures using neutron scattering, molecular dynamics simulations and quantum mechanical scattering calculations', *J. Mol. Liq.*, 290, 111168(14pp) (2019), DOI: 10.1016/j.molliq.2019.111168
- 31. F. Lique, I. Jiménez-Serra, S. Viti, **S. Marinakis***, 'Collisional excitation of PO(X) by He: New *ab initio* potential energy surfaces and scattering calculations', *Phys. Chem. Chem. Phys.*, 20, 5407-5414 (2018), DOI: 10.1039/C7CP05605B
- 30. D. Dellis, I. Samios, B. Collet, H. Versmold, J. Kłos, **S. Marinakis***, 'A computer simulation study of thermodynamics, microscopic structure, depolarized Rayleigh scattering, and collision dynamics in Xe-N₂ supercritical mixtures', *J. Mol. Liq.*, 245, 42-51 (2017) DOI: 10.1016/j.molliq.2017.06.026
- 29. G. Sarma, A. K. Saha, C. K. Bishwakarma, R. Scheidsbach, C.-H. Yang, D. Parker, L. Wiesenfeld, U. Buck, L. Mavridis, **S. Marinakis***, 'Collision energy dependence of state-to-state differential cross sections for rotationally inelastic scattering of H₂O by He', *Phys. Chem. Chem. Phys.*, 19, 4678-87 (2017) DOI: 10.1039/C6CP06495G
- 28. **S. Marinakis***, Y. Kalugina, F. Lique, 'The hyperfine excitation of OH radicals by He', *Eur. Phys.J. D*, 70, 97(7pp) (2016) DOI: 10.1140/epjd/e2016-70068-x Erratum: **S. Marinakis***, Y. Kalugina, F. Lique, 'Erratum to: The hyperfine excitation of OH radicals by He', *Eur. Phys.J. D*, 73, 92(1pp) (2016) DOI: 10.1140/epjd/e2019-100135-9
- 27. **S. Marinakis***, I. L. Dean, J. Kłos, F. Lique, 'Collisional excitation of CH(X²Π) by He: New *ab initio* potential energy surfaces and scattering calculations', *Phys. Chem. Chem. Phys.*, 17, 21583-93 (2015) DOI: 10.1039/C5CP03696H
- 26. R. Hockley, H. Irshad, T. S. Sheriff, M. Motevalli, **S. Marinakis***, 'Crystal structure of bromidonitrosylbis(triphenylphosphane-κ*P*)nickel(II)', *Acta Cryst. E71*, m87-8 (2015) DOI: 10.1107/S2056989015004703
- 25. G. Sarma, A. K. Saha, J. J. ter Meulen, D. H. Parker, **S. Marinakis***, 'Differential and integral cross sections in OH(X) + Xe collisions', *J. Chem. Phys.* 142, 034309(7pp) (2015) DOI: 10.1063/1.4906070
- 24. Y. Kalugina, F. Lique, **S. Marinakis***, 'New *ab initio* potential energy surfaces for the rovibrational excitation of OH(X²Π) by He', *Phys. Chem. Chem. Phys.* 16, 13500-7 (2014) DOI: 10.1039/C4CP01473A
- 23. M.-L. Dubernet* *et al.*, 'BASECOL2012: A Collisional Database Repository and Web Service within the VAMDC', *Astron. Astrophys.*, 553, A50(14pp) (2013) DOI: 10.1051/0004-6361/201220630

- 22. O. Denis-Alpizar, T. Stoecklin*, P. Halvick, M.-L. Dubernet, **S. Marinakis**, 'Potential energy surface and rovibrational energy levels of the H₂-CS van der Waals complex', *J. Chem. Phys.*, 137, 234301(7pp) (2012) DOI: 10.1063/1.4771658
- 21. M. Brouard, H. Chadwick, Y.-P. Chang, B. J. Howard, **S. Marinakis***, N. Screen, S. A. Seamons, A. La Via, 'Hyperfine structure of $NO(A^2\Sigma^+)$ ', *J. Mol. Spec.*, 282, 42-9 (2012) DOI: 10.1016/j.jms.2012.11.003
- G. Sarma, S. Marinakis, J. J. ter Meulen, D. H. Parker*, K. G. McKendrick, 'Velocity-Map Imaging of Hydroxyl: Inelastic scattering with Ar and He', *Nature Chem.* 4, 985-9 (2012) DOI: 10.1038/nchem.1480
- 19. **S. Marinakis***, B. J. Howard, F. J. Aoiz, J. Kłos, 'Product rotational alignment in NO(X) + Kr collisions', *Chem. Phys. Lett.* 512, 161-6 (2011) DOI: 10.1016/j.cplett.2011.07.011
- 18. G. Paterson, **S. Marinakis**, M. L. Costen, K. G. McKendrick*, J. Kłos, R. Toboła, 'Erratum: Orientation and alignment depolarisation in OH(X²Π) + Ar/He collisions', *J. Chem. Phys.* 131, 159901(3pp) (2009) DOI: 10.1063/1.3243457
- 17. F. J. Aoiz, J. E. Verdasco, M. Brouard*, J. Kłos, S. Marinakis, S. Stolte, 'Inelastic scattering of He atoms and NO(X²Π) molecules: The role of parity on the differential cross section', *J. Phys. Chem. A* 113, 14636(14pp) (2009) DOI: 10.1021/jp9043732
- 16. G. Paterson, **S. Marinakis**, M. L. Costen, K. G. McKendrick*, 'Depolarisation of rotational orientation and alignment of OH(²Π) in collisions with molecular partners: N₂ and O₂', *Phys. Chem. Chem. Phys.* 11, 8813(8pp) (2009) DOI: 10.1039/B909051G
- 15. G. Paterson, S. Marinakis, J. Kłos, M. L. Costen, K. G. McKendrick*, 'Depolarisation of rotational orientation and alignment in OH(²Π) + Xe collisions', *Phys. Chem. Chem. Phys.* 11, 8804(9pp) (2009) DOI: 10.1039/B909050A
- 14. G. Paterson, **S. Marinakis**, M. L. Costen, K. G. McKendrick*, 'Depolarisation of rotational angular momentum in open-shell collisions: OH + rare gases', *Phys. Scripta* 80, 048111(7pp) (2009) (by invitation) DOI: 10.1088/0031-8949/80/04/048111
- 13. M. Brouard*, A. Bryant, Y.-P. Chang, R. Cireasa, C. J. Eyles, A. Green, **S. Marinakis**, F. J. Aoiz, J. Kłos, 'Collisional depolarisation of OH(A) with Ar: experiment and theory', *J. Chem. Phys.* 130, 044306(12pp) (2009) DOI: 10.1063/1.3061551
- 12. G. Paterson, **S. Marinakis**, M. L. Costen, K. G. McKendrick*, J. Kłos, R. Toboła, 'Orientation and alignment depolarisation in OH(X²Π) + Ar/He collisions', *J. Chem. Phys.* 129, 074304 (18pp) (2008) DOI: 10.1063/1.2967861
- 11. M. L. Costen, **S. Marinakis**, K. G. McKendrick*, 'Do vectors point the way to understanding energy transfer in molecular collisions?', *Chem. Soc. Revs* (by invitation) 37, 732-743 (2008) DOI: 10.1039/B618070C
- 10. M. Chalaris, **S. Marinakis***, D. Dellis, 'Temperature effects on the structure and dynamics of liquid dimethyl sulfoxide: A molecular dynamics study', *Fluid Phase Equilib*. 267, 47-60 (2008) DOI: 10.1016/j.fluid.2008.02.019
- 9. **S. Marinakis**, G. Paterson, G. Richmond, M. Rockingham, M. L. Costen, K. G. McKendrick*, 'Rotational angular momentum polarisation: The influence of stray magnetic fields', *J. Chem. Phys.* 128, 021101(4pp) (2008) DOI: 10.1063/1.2829111
- 8. **S. Marinakis**, G. Paterson, J. Kłos, M. L. Costen, K. G. McKendrick*, 'Inelastic scattering of OH(X²Π) with Ar and He: A combined polarisation spectroscopy and quantum scattering study', *Phys. Chem. Chem. Phys.* 9, 4414-4426 (2007) (by invitation) DOI: 10.1039/B703909C
- 7. J. Kłos, F. J. Aoiz, J. E. Verdasco, M. Brouard*, **S. Marinakis**, S. Stolte, 'Fully quantum state-resolved inelastic scattering between He and NO(X ²Π)', *J. Chem. Phys.* 127, 031102(4pp) (2007) DOI: 10.1063/1.2756826
- 6. M. Brouard*, A. Bryant, I. Burak, **S. Marinakis**, F. Quadrini, I. Garcia, C. Vallance, 'Collisional depolarisation of OH(A) studied by Zeeman quantum beat spectroscopy', *Molec. Phys.* 103, 1693-1702 (2005) DOI: 10.1080/00268970500096293
- 5. **S. Marinakis***, I. Samios, 'The temperature and density dependence of fluid xenon self-diffusion coefficients: a comparison between experimental, theoretical and molecular dynamics results', *J. Supercrit. Fluids* 34, 81-9 (2005) DOI: 10.1016/j.supflu.2004.10.002
- 4. M. Brouard*, I. Burak, **S. Marinakis**, L. Rubio Lago, P. Tampkins, C. Vallance, 'Product spin-orbit dependence of the H + H₂O and H + D₂O abstraction reactions', *J. Chem. Phys.* 121, 10426-10436 (2004) DOI: 10.1063/1.1809578
- 3. M. Brouard*, **S. Marinakis**, L. Rubio Lago, F. Quadrini, D. Solaiman, C. Vallance, F. J. Aoiz, L. Bañares, J. F. Castillo, 'Cross-sections for the H + H₂O→OH + H₂ and H +

- $D_2O \rightarrow OD + HD$ abstraction reactions', *Phys. Chem. Chem. Phys.* 6, 4991-9 (2004) DOI: 10.1039/B409667C
- 2. M. Brouard*, I. Burak, **S. Marinakis**, D. Minayev, P. O' Keeffe, C. Vallance, F. J. Aoiz, L. Bañares, J. F. Castillo, D. H. Zhang, D. Xie, M. Yang, S. Y. Lee, M. A. Collins, 'Cross section for the H + H₂O abstraction reaction: experiment and theory', *Phys. Rev. Lett.* 90, 093201-4 (2003) DOI: 10.1103/PhysRevLett.90.093201
- 1. **S. Marinakis***, I. Kerkines, 'Chemical Warfare Agents', *Greek Military Review*, 5, 106-121 (2002)

TRANSLATIONS

C. Garoufalis, S. Marinakis, 'Python για Χημικούς', (in Greek), Gotsis Publications, Patras (2025) [Original book: C. Hill, Python for Chemists, Cambridge University Press, Cambridge (2024)].

BOOKS

1. E. Dalas, A. Chrysanthopoulos, S. Dionysopoulou, **S. Marinakis***, D. Sevastos, 'Laboratory Exercises in Experimental Physical Chemistry' (in Greek), University of Patras, Patras, 152 pp (2022) (co-authored and editor).

ABSTRACTS IN CONFERENCES

- P. Leventis, N. N. Lathiotakis, S. Marinakis, 'Electronic and magnetic properties of Prussian Blue studied with periodic DFT' (in Greek), 14ο Πανελλήνιο Επιστημονικό Συνέδριο Χημικής Μηχανικής, Θεσσαλονίκη, 29-31 Μαΐου 2024, 809-814.
- P. Marouli, P. D. Natsi, I. Tzoumani, S. Marinakis, E. Dalas, P. G. Koutsoukos, 'Study of calcification of polymeric materials with antimicrobial activity (in Greek)', 14ο Πανελλήνιο Επιστημονικό Συνέδριο Χημικής Μηγανικής, Θεσσαλονίκη, 29-31 Μαΐου 2024, 834-839.

OUTREACH

- 22. 'The 2nd International Conference on Physical Chemistry and Spectroscopy' (in Greek), UP: Περιοδική Έκδοση Πανεπιστημίου Πατρών, Τεύχος 15, σελίδες 9-10, Νοέμβριος Δεκέμβριος 2023, https://www.upatras.gr/wp-content/uploads/2023/12/@up15.pdf
- 21. Local co-organizer for RSC Top of the Bench final (University of East London, September 2020)
- 20. Local organizer for an outreach event with Dr David Peggie of the National Gallery (University of East London, March 2020)
- 19. Speaker and local organizer for 'Raising awareness of STEM careers through STEM teaching' for teachers with the Royal Academy of Engineering, Pedagogics, EastLondonScience (University of East London, July 2019)
- 18. STEM and Chemistry event for Year 9 Students (laboratory exercise and organizer) with the Royal Academy of Engineering, Pedagogics, EastLondonScience (University of East London, July 2019)
- 17. Royal Docks Education and Enterprise Festival (University of East London, June 2019)
- 16. Salters Festival (University of East London, May 2019)
- 15. Outreach event / laboratory exercise with New City College year 11-12 students (University of East London, April 2019)
- 14. Outreach event with Royal Society of Chemistry (Cambridge Science Festival, Cambridge, March 2019)
- 13. Local organizer for the Royal Society of Chemistry 'Microscale workshop' for chemistry teachers (University of East London, January 2019)
- 12. 'Teaching mathematics for chemistry students: high school and higher education' (talk, and local organizer for the Royal Society of Chemistry workshop 'Teaching numeracy in

- Chemistry to improve outcomes in the classroom', University of East London, December 2018)
- 11. Outreach event with Royal Society of Chemistry (Basildon Street Science Festival, Essex, September 2018)
- 10. Outreach talk for sixth form college students (Woodhouse College, London, July 2017)
- 9. Open day talks (Queen Mary, London, June 2017)
- 8. S. Marinakis, B. J. Howard (2015) *Microwave radiation*, podcast audio program. Available at http://qmro.qmul.ac.uk/xmlui/handle/123456789/9475 DOI: 10.17636/01009475
- 7. S. Marinakis, B. J. Howard (2015) *Microwave studies of nitrosyl complexes*, podcast audio program. Available at http://qmro.qmul.ac.uk/xmlui/handle/123456789/9476 DOI: 10.17636/01009476
- 6. S. Marinakis, B. J. Howard (2015) *Setting the problem*, podcast audio program. Available at http://qmro.qmul.ac.uk/xmlui/handle/123456789/9477 DOI: 10.17636/01009477
- 5. S. Marinakis, B. J. Howard (2015) *Experimental and theoretical approaches*, podcast audio program. Available at http://qmro.qmul.ac.uk/xmlui/handle/123456789/9478 DOI: 10.17636/01009478
- 4. S. Marinakis, B. J. Howard (2015) *Possible health effects of magnetic fields*, podcast audio program. Available at http://qmro.qmul.ac.uk/xmlui/handle/123456789/9479 DOI: 10.17636/01009479
- 3. S. Marinakis, B. J. Howard (2015) *What does the future hold for microwave? 'Microwave effect'*, podcast audio program. Available at http://gmro.gmul.ac.uk/xmlui/handle/123456789/9480 DOI: 10.17636/01009480
- 2. S. Marinakis, B. J. Howard (2015) *What does the future hold for microwave? Medicine*, podcast audio program. Available at http://qmro.qmul.ac.uk/xmlui/handle/123456789/9481 DOI: 10.17636/01009481
- 1. Outreach talk for secondary school pupils (Greek Secondary School of London, May 2015)