Stefan T. Bromley

Personal Details

Date, place of birth:	23rd November, 1971, Loughborough, U.K.
Family status:	Married (3 children)
Language skills:	English, Spanish
Official address:	Departament de Química Física, Universitat de Barcelona, c/ Marti i Franques, 1, 08028 Barcelona, Spain Tel. (+34) 93 403 9266, Fax (+34) 93 402 1231 E-mail: s.bromley@ub.edu Website: www.ub.edu/nnmgroup

Education

1990 – 1994	BSc Honours in Theoretical Physics (graded 1st), University of St. Andrews, U.K. Final year project "Causal Interpretation of Quantum Mechanics" (graded 1st).
1994 – 1997	Doctorate (PhD) in Computational Physics: A Monte Carlo study of pairing mechanisms in high temperature superconductors, University of Southampton, UK.

Employment History

1997 – 1999	Postdoctoral Researcher in project "Bimetallic Nanoparticles Anchoured in Nanoporous Hosts", The Royal Institution of Great Britain (RIGB), London, UK.
1999 – 2000	Research member of EU academic/industrial ESPRIT project: "QUASI-Quantum Simulation in Industry" researching ZnO-supported nanoclusters, RIGB, London (UK).
2000 – 2004	Associate Professor and group leader of the Computational Chemistry group at Delft University of Technology – TUDelft, The Netherlands.
2004 – 2007	"Ramón y Cajal" Research Fellow within the Quantum Chemistry of Materials group, Dept. of Physical Chemistry, University of Barcelona (UB), Spain.
2007 – now	Research Professor, ICREA (Catalan Institute of Research and Advanced Studies) heading the "Nanoclusters and Nanostructured Materials" group in the Dept. of Physical Chemistry / Institute of Computational and Theoretical Chemistry (IQTC), UB, Spain.

Scientific production summary

Number of PhD theses directed to completion: 13 (currently supervising 7 PhD students)
Number of Masters theses directed to completion: 7 (currently supervising 2 Masters students)
Total citations: >8000 (Scopus/Web of Science) / >10000 (Google Scholar)
Av. number of citations per year (last 5 years): 512 (ISI Web of Science) / 627 (Google Scholar)
First and/or corresponding author on ~70% of publications
Number of publications: > 200
h-index: 47 (Scopus/Web of Science) / 53 (Google Scholar)
Book chapters: 8
Books edited: 2
Invited oral presentations: >80
Researcher ID: A-2481-2009
ORCID code: 0000-0002-7037-0475

Career Summary

Stefan T. Bromley (1971) started his professional research career with three years as a postdoctoral fellow (1997-2000) modelling oxide-supported metal nanoclusters at the Royal Institution of Great Britain (RIGB, UK), with Prof. C. Richard Catlow. The project involved a strong collaboration with heterogeneous catalysis experiments at Cambridge University (Profs. Brian Johnson and John M. Thomas). Later, the modelling of these systems was more strongly linked to industrial applications through an EU-funded project (QUASI-Quantum Simulation in Industry).

In 2000 STB obtained an Associate Professorship at the Technical University of Delft (TUDelft, The Netherlands) where he formed his own Computational Chemistry group. Following experience at RIGB and the research interests at TUDelft, the group focussed its efforts on nanostructured and nanoscale silicates which have huge industrial importance (e.g. zeolites for catalysis and separation). The group (2 PhD students, 2 Postdocs) published many important articles on the fundamental understanding of nanosilica,

and in particular on the potential use of nanoporous sllicates for hydrogen storage. Funding for one of the postdocs was obtained through a project funded by the oil company Shell.

In 2004 STB moved to the University of Barcelona (UB) with a tenure track Ramon y Cajal fellowship with a project on modelling nanosilicates. Initially, he worked with the group of Prof. Francesc Illas where his experience with modelling nanomaterials and catalytic systems matched the group's main focus on surface science and heterogeneous catalysis. In 2007 STB became a Research Professor with the Catalan Institution for Research and Advanced Studies (ICREA) and formed the Nanoclusters and Nanostructured Materials (NNM) group (see: www.ub.edu/nnmgroup). The NNM group is an independent group within the Institute of Computational and Theoretical Chemistry at the UB. Initially the main research focus of the NNM group concerned Inorganic Nanomaterials, but the group now increasingly works on Organic Electronics/Spintronics and Astro/nanomineralogy - often with external collaborators. An overview of work in these three research lines can be found below.

STB has supervised 7 Master students,13 PhD students and 6 Postdocs. Of these, 3 went on to obtain prestigious fellowships (Marie Curie, Humbolt, EPSRC) and 3 of which now have permanent academic positions: Dr. M. A. Zwijnenburg, Professor at University College London (UK), Dr. Edwin Flikkema, Lecturer at Aberystwyth (UK), Dr. Naseem Ramsahye, Lecturer at Ecole Nationale Supérieure de Chimie de Montpellier (France). STB is on the editorial board of the journal "Inorganics" and regularly assists on the advisory/evaluation panels for high performance computing resources ("Chemistry and New Materials" Panel for the Red Española de Supercomputacion – 2014-2016, International assessment Panel to assess current and future directions of the UK´s HEC Materials Chemistry Consortium – 2012 & 2016).

Representative publications (full list: https://scholar.google.com/citations?user=GRcDA5cAAAAJ&hl=en)

IF = journal impact factor / **COLL** = collaboration with external research groups

Books, special issues & reviews:

1. **Book:** S. T. Bromley & S. M. Woodley (Eds.) (2018) **Computational Modelling of Nanoparticles**, Frontiers in Nanoscience Vol. 12, Elsevier. ISBN: 9780081022757.
   - Introduction to modelling inorganic nanoclusters with a varied range of examples.

2. **Book:** S. T. Bromley & M. A. Zwijnenburg (Eds.) (2016) **Computational Modeling of Inorganic Nanomaterials** CRC Press. ISBN: 9780429194184.
   - Structured intrduction to modelling inorganic nanomaterials with a range of dimensionalities together with selected pertinent case studies.

3. **Special Issue:** R. C. Fortenberry & S. T Bromley (Eds.) (2022) **Refractory Astrochemistry**, *Front. Astron. Space Sci.* 9, 859101 https://doi.org/10.3389/fspas.2022.859101
   - Selected invited papers covering modelling and observations of cosmic dust materials.

4. **Special Issue:** S. T. Bromley & S. M. Woodley (Eds.) (2016) **Inorganic Nanoclusters: Advances in Understanding Structure and Properties**, *Inorganics*, www.mdpi.com/journal/inorganics/special_issues/inorganic_nanoclusters
   - Selected invited papers covering both experimental and theoretical studies of inorganic nanoclusters.

5. **Review:** A. Potapov, M. R. S. McCoustra, R. Tazaki, E. A. Bergin, S. T. Bromley, R. T. Garrod, A. Rimola (2025) **Is cosmic dust porous?** *Astron. Astrophys. Rev.* 33, 1. **IF**=26.5 **COLL**
   - Detailed review of the evidence and role of porosity in cosmic dust particles.

6. **Review:** I. Ratera, J. Vidal-Gancedo, D. Maspoch, S. T. Bromley, N. Crivillers, M. Mas-Torrent (2021) **Perspectives for polychlorinated trityl radicals** *J. Mater. Chem. C*, 9, 10610. **IF**=5.2 **COLL**
   - Overview the recent and prospective applications of persistent trityl radicals

7. **Review:** S. T. Bromley, (2025) **Nanosilicates and molecular silicate dust species: properties and observational prospects** *Front. Astron. Space Sci.* 11, 1523977 **IF**=2.6
   - Concise review of the evidence for nanosilicates in various astrophysical environments.

8. **Review:** S. T. Bromley, I. de P. R. Moreira, K. M. Neyman, F. Illas, (2009) **Approaching nanoscale oxides: models and theoretical methods**, *Chem. Soc. Rev.* 38, 2657. **IF**=40.4
   - Detailed review of the challenges involved in modelling nanoscale oxides.

9. **Review:** S. T. Bromley, T. P. M. Goumans, E. Herbst, A. P. Jones and B. Slater (2014) **Challenges in modelling the reaction chemistry of interstellar dust**, Phys. Chem. Chem. Phys. (Perspective), 74, 58. **IF**=3.4. **COLL**.
   - Review of a range of state-of-the-art approaches to model the properties and chemistry of interstellar dust

10. **Review:** C. R. A. Catlow, S. T. Bromley, S. Hamad, M. Mora-Fonz, A. A. Sokol, S. Woodley (2010) **Modelling nano-clusters and nucleation**, Phys. Chem. Chem. Phys. (Perspective) 12, 786. **IF**=3.4. **COLL**.
   - Overview of methods to model inorganic nanoclusters with pertinent case studies.

Research Articles (10 selected for each research line) – underlining denotes corresponding authors

Organic Electronics/Spintronics (Focus on 2D materials based on persistent radicals)**:**

1. K. Jutglar-Lozano, M. Deumal, J. Ribas-Arino, S. T. Bromley (2025) **Rational Design of Electric Field-Responsive Building Blocks for All-Organic 2D Magnetoelectric Materials** J. *Am. Chem. Soc.* 147, 22550 **IF**=15.7
   - We show how to design fully organic 2D magnetoelectric materials using dipolar twistable linkers.

2. I. Alcón, J. Ribas-Ariño, I. de P. R. Moreira, S. T. Bromley (2023), **Emergent spin frustration in neutral mixed-valence 2D conjugated polymers: A potential quantum materials platform**, J. *Am. Chem. Soc.* 145, 5674. IF=15.7
   - We show that substitution with B or N can yield spin frustation in 2D covalent organic radical materials leading to a viable platform for designing quantum materials.

3. I. Alcón, R. Santiago, J. Ribas-Arino, M. Deumal, I. de P. R. Moreira, S. T. Bromley, **Controlling pairing of π-conjugated electrons in 2D covalent organic radical frameworks via in-plane strain** (2021) *Nat. Commun.* 12, 1705. **IF**=15.7
   - We show that in-plane tension can control electron pairing in 2D covalent organic radical materials.

4. R. Santiago, I. Alcón, J. Ribas-Arino, M. Deumal, I. de P. R. Moreira, S. T Bromley (2020) **2D Hexagonal Covalent Organic Radical Frameworks as Tunable Correlated Electron Systems**, *Adv. Funct. Mater.* 2004584. **IF**=19.0
   - We show that out-of-plane compression can tune the correlated electronic states of 2D covalent organic radical materials.

5. M. R. Ajayakumar, C. Moreno, I. Alcón, F. Illas, C. Rovira, J. Veciana, S. T Bromley, A. Mugarza, M. Mas-Torrent (2020) **Neutral Organic Radical Formation by Chemisorption on Metal Surfaces**, *J. Phys. Chem. Lett.* 11, 3897. **IF**=4.7 **COLL**
   - We design and demonstrate a proof-of-principle example of a neutral molecule that becomes a stable radical upon chemisorption with an approriate metal surface.

6. I. Alcón, F. Viñes, I. de P. R. Moreira, S. T. Bromley (2017) **Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials** *Nat. Commun.* 8, 1957. **IF**=15.7
   - We show that 2D covalent organic radical frameworks can be considered as extended graphene-like materials which, unlike graphene, show low lying open-shell and gapped semiconductor states.

7. I. Alcón, D. Reta, I. de P. R. Moreira, S. T. Bromley (2017) **Design of multi-functional 2D open-shell organic networks with mechanically controllable properties**, *Chem. Sci.* 8, 1027. **IF**=7.5
   - We design 2D covalent organic radical farmeworks in which modest in-plane strain is able to tune the electronic properties.

8. C. Franco, P. M. Burrezo, V. Lloveras, R. Caballero, I. Alcon, S. T. Bromley, M. Mas-Torrent, F. Langa, J. T. Lopez Navarrete, C. Rovira, J. Casado, J. Veciana (2017) **Operative mechanism of Hole-Assisted Negative charge motion in ground states of Radical-Anion molecular wires**, J. *Am. Chem. Soc.* 139, 686. **IF**=15.7 **COLL**
   - An experimental and theoretical study showing how ground state electrons move in anionic molecular wires with radical end-terminations.

9. N. Crivillers, C. Munuera, M. Mas-Torrent, C. Simão, S. T. Bromley, C. Ocal, C. Rovira, J. Veciana (2009) **"Dramatic Influence of the Electronic Structure on the Conductivity through Open- and Closed-Shell Molecules"**, *Adv. Mater.* 21, 1177. **IF**=26.8 **COLL**
   - A dramatic change in conductivity is observed and theoretically rationalised in monolayers of two structurally very similar molecules differing in their closed-shell vs open shell character.

10. S. T. Bromley, M. Mas-Torrent, P. Hadley, C. Rovira (2004) **"Importance of Intermolecular Interactions in Assessing Hopping Mobilities in Organic Field Effect Transistors: Pentacene versus Dithiophene-tetrathiafulvalene"**, *J. Am. Chem. Soc.* 126, 6544. **IF**=15.7 **COLL**
- Calculations show that the high mobility in DT-TTF is strongly dependent on the local crystal packing through its effect on the charge transfer reorganisation energy.

Cosmic dust (Focus on properties of astronomically relevant nanosilicates):

1. J. Mariñoso Guiu, A.M. Escatllar, S. T. Bromley (accepted for publication 2025) **The Nucleated Atomistic Grain Growth Simulator (NAGGS): application to the size-dependent structural and physical properties of nanosilicate dust**, *Astronom. Astrophys.* (arXiv:2601.05430). **IF**=5.8
- We introduce a new method to model realistically grown nano-sized dust grains and demonstrate the method for the case of nanosilicates.

2. J. Mariñoso Guiu, J. M. Bakker, T. M Bernhardt, J. M. C. Plane, S. T. Bromley, S. M. Lang (2025) **Oxygen-rich anionic metal silicate clusters as nucleation seeds for noctilucent clouds**, *npj Climate Atmos. Sci.* 8, 153. **IF**=8.4 **COLL**
- Using cluster beam data and a range of theoretical modelling methods we predict that anionic silicate clusters are highly credible seed species for nucleating noctilucent clouds.

3. S. T. Zeegers, J. Mariñoso Guiu, F. Kemper, J. P. Marshall, S. T. Bromley (2023) **Predicting observable infrared signatures of nanosilicates in the diffuse interstellar medium,** *Faraday Discuss.* 245, 609 **IF**=4.4 **COLL**
- Based on theoretical IR spectra of nanosilicates and estimates of the sensitivity of the James Webb Space Telescope, we predict that nanosilicates should be detectable.

4. J. Mariñoso Guiu, B-A. Ghejan, T. M. Bernhardt, J. M. Bakker, S. M. Lang, S. T. Bromley (2022) **Cluster beam study of $(MgSiO_3)^+$-based monomeric silicate species and their interaction with oxygen: implications for interstellar astrochemistry**, *ACS Earth Space Chem.* 6, 2465. **IF**=2.9 **COLL**
- In a collaborative study with cluster beam experimentalists, we reveal the structure and chemistry of pyroxene-based silicate nanoclusters.

5. A.M. Escatllar, S. T. Bromley (2020) **Assessing the viability of silicate nanoclusters as carriers of the anomalous microwave emission: a quantum mechanical study**, *Astronom. Astrophys.* 634, A77. **IF**=5.8
- From quantum chemical calculations we establish a solid basis for arguing that nanosilicates are the likely carriers of the ubiquitous anomalous microwave emission.

6. A. M. Escatllar, T. Lazaukas, S. M. Woodley, S. T. Bromley (2019) **Structure and Properties of Nanosilicates with Olivine $(Mg_2SiO_4)_N$ and Pyroxene $(MgSiO_3)_N$ Compositions,** *ACS Earth Space Chem.* 3, 2390. **IF**=2.9 **COLL**
- Based on accurate and intensive global optimization searches we establish the structures and properties of stable Mg-rich olivine and pyroxene nanoclusters.

7. L. Zamirri, A. Macia Escatllar, J. Mariñoso Guiu, P. Ugliengo, S. T. Bromley (2019) **What Can Infrared Spectra Tell Us about the Crystallinity of Nanosized Interstellar Silicate Dust Grains?**, *ACS Earth Space Chem.* 3, 2323. **IF**=2.9 **COLL**
- We show that the IR spectra of crystalline nanosilicate dust is strongly dependent on size potentially meaning that some observational IR dust spectra should be re-interpreted.

8. S. T Bromley, J. C. G. Martin, J. M. C. Plane (2016) **Under what conditions does $(SiO)_N$ nucleation occur? A bottom-up kinetic modelling evaluation**, *Phys. Chem. Chem. Phys.* 18, 26913. **IF**=3.7. **COLL**
- Using the free energies of globally optimised $(SiO)_N$ clusters and kinetic modelling a bottom-up prediction of the temperature/pressure dependency of SiO nucleation is reported.

9. B. Kerkeni, S. T. Bromley (2013) **Competing Mechanisms of Catalytic H_2 Formation and Dissociation on ultrasmall silicate nanocluster dust grains**, *Mon. Not. R. Astron. Soc.* 435, 1486. **IF**=4.8. **COLL**.
- Exploration of the interaction of H atoms and molecular hydrogen formation on a nanosilicate with forsterite composition.

10. T. P. M. Goumans, S. T. Bromley (2012) **Efficient Nucleation of Stardust Silicates via Heteromolecular Homogeneous Condensation**, *Mon. Not. R. Astron. Soc.* 420, 3344. **IF**=4.8. **COLL**.
    - First ever detailed atomistic account of how silicate dust could efficiently form around AGB stars.

Inorganic nanomaterials (Focus on technologically important reducible nano-oxides)**:**

1. M. Recio-Poo, C. H. Rotteger, F. Illas, S. T. Bromley, A. Morales-García, S. C. Sayres, A. V. Akimov (2026) **Revealing Recombination and Ultrafast Relaxation Mechanisms in Atomically Precise Titania Nanoclusters**, *J. Am. Chem. Soc.* 147, 40900. **IF**=15.7
    - In an international experimental/theoretical collaboration we reveal the subtle difference in timescales between different excited state relaxation mechanisms.

2. M. Recio-Poo, A. Morales-García, F. Illas, S. T. Bromley (2024) **Tuning electronic levels in photoactive hydroxylated titania nanosystems: combining the ligand dipole effect and quantum confinement**, *Nanoscale* 16, 8975. **IF**=5.1
    - We show how electronic levels in titanis nanoparticles can be tuned by their size and degree of hydroxylation.

3. G. Di Liberto, A. Morales-García, S. T. Bromley (2022) **An unconstrained approach to systematic structural and energetic screening of materials interfaces**, *Nat. Commun.* 13, 6236. **IF**=15.7
    - We introduce a new method to screen the stability of materials interfaces using rotating nanosized disks.

4. Á. Morales-García, A. M. Escatllar, F. Illas, S. T. Bromley (2019) **Understanding the interplay between size, morphology and energy gap in photoactive TiO_2 nanoparticles,** *Nanoscale* 11, 9032. **IF**=5.1
    - By considering a range of nanoparticle types we establish a predictive phase diagram of how morphology, size and crystallinity affect the band gap in nano-TiO_2.

5. O. Lamiel-Garcia, A. Cuko, M. Calatayud, F. Illas, S. T. Bromley (2017) **Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals,** *Nanoscale* 9, 1049. **IF**=5.1 **COLL**
    - Comparing top-down and bottom-up generated nanoparticles we predict the size at which bulk-like crystallinity becomes more stable than amorphous non-bulk structures.

6. F. Viñes, O. Lamiel-Garcia, F. Illas, S. T. Bromley (2017) **Size dependent structural and polymorphic transitions in ZnO: from nanocluster to bulk,** *Nanoscale* 9, 10067. **IF**=6.9
    - Comparing nanoparticles and bulk phases of stable ZnO polymorphs we show how polymorphic stability depends on size.

7. I. Demiroglu, S. M. Woodley, A. A. Sokol, S. T. Bromley, (2014) **"From monomer to monolayer: a global optimisation study of $(ZnO)_n$ nanoclusters on the Ag surface"**, *Nanoscale* 6, 14754. **IF**=6.9. **COLL**
    - The evolution of a supported oxide material from monomer to monolayer is modelled for the first time for the important wide-band gap semiconductor ZnO.

8. I. Demiroglu, S. T. Bromley, (2013) **Nanofilm versus Bulk Polymorphism in Wurtzite Materials,** *Phys. Rev. Lett.* 110, 245501. **IF**=8.4
    - The relative stability of different crystal polymorphs is shown to be intrinsically linked to whether material is a bulk phase or possesses nanoscale dimensions.

9. M. A. Zwijnenburg, F. Illas, S. T. Bromley (2010) **Apparent scarcity of low-density polymorphs of inorganic solids,** *Phys. Rev. Lett.* 104, 175503. **IF**=8.4
    - Extensive calculations highlighting that many, as-yet unsynthesised, low density materials are likely to be structurally and energetically stable polymorphs.

10. J. Carrasco, F. Illas, S. T. Bromley, (2007**) Ultralow-density nanocage-based metal-oxide polymorphs**, *Phys. Rev. Lett.* 99, 235502. **IF**=8.4
    - Prediction of novel nanoporous oxide materials based on nanocage building blocks viability with respect to known synthesized materials.

Recent Involvement in Funded Research Projects **(10 selected)**

1. **Title:** Atomistic Modeling of the Physicochemical Properties of Interstellar Dust Grains
   Principal Investigator: Stefan Bromley

Funding source: Spanish Ministry of Science, Innovation and Universities (MICIU)
Reference: PID2024-157971NB-C22
Initial/final date: 2025-2028
Total awarded: € 102500

2. **Title:** Towards Efficient Hydrogen Production with New Hybrid Electrocatalysts (HYDROCAT)
   Principal Investigator: Stefan Bromley
   Funding source: Generalitat de Catalunya
   Reference: 2023 CLIMA 00064
   Initial/final date: 2024-2026
   Total awarded: €120000

3. **Title:** Computational design of hybrid Metal-Organic Radical ElectroCATalysts for reactions of socioeconomic and environmental importance (MORECAT)
   Principal Investigator: Stefan Bromley
   Funding source: Spanish Ministry of Science, Innovation and Universities (MICIU)
   Reference: PID2021-127957NB-I00
   Initial/final date: 2022-2026
   Total awarded: €163,350

4. **Title:** Electrocatalysts based on Redox Active Self Assembled Monolayers (ERASAM)
   Principal Investigator: Stefan Bromley
   Funding source: Spanish Ministry of Science, Innovation and Universities (MICIU) + EU
   Reference: TED2021-132550B-C21
   Initial/final date: 2022 - 2025
   Total awarded: € 132480

5. **Title:** Th**e** Novel Materials Discovery (NoMaD) Laboratory
   Principal Investigator: Matthias Scheffler
   Funding source: Horizon 2020 – European Comission
   Reference: 676580 – NoMaD – H2020-EINFRA-2014-2015
   Initial/final date: 2015 - 2018
   Total awarded: € 4910624

6. **Title:** Theoretical Chemistry and Computational Modelling Innovative Training Network
   Principal Investigator: Manuel Yañez
   Funding source: Horizon 2020 – European Comission
   Reference: ITN-EJD-TCCM
   Initial/final date: 2015 - 2018
   Total awarded: € 3785868

7. **Title:** Knowledge Led Structure Prediction for Nanostructures
   Principal Investigator: Scott Woodley
   Funding source: Engineering and Physical Sciences Research Council (EPSRC), UK
   Reference: EP/K038958/1
   Initial/final date: 2013 - 2018
   Total awarded: € 1082000

8. **Title:** Unidades de Excelencia María de Maeztu: INSTITUT DE QUIMICA TEORICA I COMPUTACIONAL (IQTC)
   Principal Investigator: Eliseo Ruiz
   Funding source: Ministerio de Ciencia e Innovacion, Spain
   Reference: CEX2021-001202-M
   Initial/final date: 2022 - 2026
   Total awarded: € 2000000

9. **Title:** Understanding, controlling, and optimizing heterogeneous catalysts and photocatalysts at the nanoscale. Application to carbon dioxide conversion and hydrogen production
   Principal Investigators: Stefan Bromley & Francesc Illas
   Funding source: Ministerio de Economía y Competitividad, Spain
   Reference: Initial/final date: 2016 - 2019
   Total awarded: € 164560

10. **Title:** Modelling Mixed-Oxide Materials with Technological and Environmental Relevance
    Principal Investigator: Stefan Bromley
    Funding source: Ministerio de Economía y Competitividad, Spain
    Reference: MAT2012-30924
    Initial/final date: 2013 - 2015
    Total awarded: € 38025

Conference Organisation

1. Organised workshop (with F. Goumans and B. Slater): “Challenges in Modelling the Reaction Chemistry of Interstellar Dust”, Lorentz Center, Leiden, The Netherlands (Sept. 2011).

2. Co-organiser: “Theoretical Modelling of Materials”, a satellite meeting of the World Association of Theory Oriented Chemists”, WATOC 2011, Barcelona July 13-15, 2011.

3. Organised workshop (with M. A. Zwijnenburg): Modelling Realistic Inorganic Nanostructures: Bridging the Gap between Theory and Experiment, Z-CAM, Zaragoza, Spain (Sept. 2012).

4. Co-organiser: Transparent Conducting Oxides Symposium, European Materials Research Society (EMRS) Fall Meeting, Warsaw, Poland (Sept. 2014)

5. Organised and chaired workshop (with J. Matxain): “iPolymorphs: Novel routes to new inorganic polymorphs”, San Sebastian, Spain (Jun. 2016).

6. Organised and chaired “Chemistry and New Materials” session of Jornada de Usuarios de la RES (Spanish Supercomputing Network), Leon, Spain (Sept. 2016).

Selected oral presentations (5 selected for each research line from >80 given during full career)

Organic Electronics/Spintronics

Invited: "Towards new 2D quantum materials from single-layer chemically-expanded graphenic lattices" - Graphene2024 Conference, Madrid (Spain, 2024).
Invited: "From Molecular Radicals to 2D Quantum materials: 2D Covalent Organic Radical Frameworks", Chem2Dmat - European Conference on Chemistry of 2D Materials, Bologna (Italy, 2023).
Invited: 'From Gomberg to graphene and beyond: new multifunctional 2D materials based on persistent radicals', Royal Society Hooke Discussion Meeting, Supercomputer modelling of advanced materials, The Royal Society, London (UK, 2022)
Invited: “Post-graphene organic Dirac materials with tunable spin-polarised and closed-shell semiconducting states”, Graphene2018 conference, San Sebastian, (Spain, 2018).
Invited: “Design of open-shell 2D covalent materials with controllable properties”, European Materials Research Symposium (E-MRS) Spring Meeting, Lille (France, 2016).

Cosmic Dust

Invited: “Understanding Trapped Molecular Water on Silicate Grain Surfaces”, European Conference on Surface Science - ECOSS 38, Braga (Portugal, 2025).
Invited: “Assessing the astronomical relevance of interstellar nanosilicate dust grains from IR spectra: theory, experiment and observation”, Conference on “Origin and Fate of Dust in our Universe”, Goteburg (Sweden 2023).
Invited: 'Nanosilicate Dust in the Interstellar Medium: Theory, Experiment and Obervation', Collision Physics and Chemistry and their Applications Conference, COPCA 2022 Valletta (Malta, 2022)
Invited: “Using atomistically detailed simulations to understand the formation, structure and composition of astrophysical silicate dust grains”, International Astronmical Union Symposium on Laboratory Astrophysics: from Observations to Interpretation, Cambridge (UK, 2019).
Invited: “A Bottom-up Computional Modelling Approach to the Formation and Properties Silicate Dust”, Gas on the Rocks, European Conference on Laboratory Astrophysics - ECLA 2016, Madrid (Spain, 2016).

Inorganic Nanomaterials

Invited: “Effect of size and hydroxylation on the structure and reactivity of oxide nanoparticles”, International Workshop & NIS colloquium on Heterogeneous catalysis based on naturally occurring materials: from prebiotic chemistry to applications, Torino (Italy, 2023).
Invited: “Understanding the Interplay between Size, Morphology and Energy Gap in Photoactive TiO_2 Nanoparticles”, European Materials Research Society (E-MRS Fall meeting), Warsaw (Poland, 2019).
Invited: “Tracking the Properties of Oxide Materials from Nanoscale to Bulk”, Multi-Scale Modelling Track, IEEE Nano, Cork (Ireland, 2018).

Keynote: “Nanocrystals versus Nanoclusters, Limits on Crystallinity and Small Size”, British Association of Crystal Growth Meeting, London (UK, 2015)
Keynote: “Nanoscale Ceria: What Can Computational Modelling Tell Us?”, World Resources Forum, National Conference Center, Beijing, (China, 2012).

Participation in advisory/examination panels

2014-2016: Member of the “Chemistry and New Materials” panel for the access committee to the Spanish Supercomputing Network (RES).

2012 and 2016: Advisory panel member to the “High Performance Computing Materials Chemistry Consortium”, UK

2010-2015: Member of examination committee for six PhD defenses in 3 Spain, 1 France, 1 Switzerland and 1 UK.

Industrial collaborations/contracts/patents

2025 - : Inventor on an interational patent (WO2025229053 - VACANCIES IN CARBON-BASED 2D LAYERS AND CARBON-BASED STRUCTURES). The patent has been licenced by the company Ideaded.

2003 - 2004: secured 60000 Euros project funding from Shell Chemicals (Amsterdam, NL) for modelling project: “Understanding Double Metal Catalysts for Propoxylation”.

1999 - 2000: Member of European Union funded Academic/Industrial ESPRIT project: “QUASI-Quantum Simulation in Industry”, EP25047. Involved development of user-friendly software for realistic modelling of catalytic systems and the transfer this technology to industrial partners (BASF, Norsk Hydro, ICI Chemicals). See: http://cordis.europa.eu/esprit/src/25047.htm

Research collaborations

Prof. C. Richard Catlow, University College London, UK
Dr. Scott Woodley, University College London, UK
Prof. Jaume Veciana, Institut de Ciencia de Materials de Barcelona, Spain
Prof. Piero Ugliengo, University of Turin, Italy
Prof. Aitor Murgaza, Catalan Institute of Nanoscience and Nanotechnology, Spain
Prof. John Plane, University of Leeds, UK
Prof. Monica Calatayud, University Pierre et Marie Curie, France
Prof. Thomas Henning, Max Planck Institute for Astronomy, Germany
Dr. Cornelia Jaeger, University of Jena, Germany
Dr. Sandra Lang, Ulm University, Germany
Dr. Ciska Kemper, Academia Sinica Institute of Astronomy and Astrophysics, Taiwan
Prof. Isabelle Cherchneff, University of Basel, Switzerland
Dr. Christiane Helling, University of St. Andrews, UK
Prof. Christian Schoen, Max Planck Institute for Solid State Research, Germany
Dr. Boutheina Kerkeni, University Pierre et Marie Curie, France
Prof. Jumras Limtrakul, Kasetsart University, Thailand
Prof. Bernd Hartke, University of Kiel, Germany
Prof. Peter Sushko, Pacific Northwest National Laboratory, USA
Dr. Lorenzo Mino, University of Torino, Italy
Dr. Giovanni di Liberto, University of Milan Bicocca, Italy
Dr. Alexey Akimov, University at Buffalo, USA
Dr. Scott Sayres, Pennsylvania State University

Reviewing for journals

Nature Materials, Nature Catalysis, Proceedings of the National Academy of Sciences of the USA, Advanced Materials, Advanced Functional Materials, Angewandte Chemie, ACS Nano, Nano Letters, Journal of the American Chemical Society, Physical Review Letters, Chemical Science, Nanoscale, Journal of Physical Chemistry (A, B, C and Letters), Chemical Communications, Chemistry of Materials, Journal of Materials Chemistry, ChemPhysChem, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Physical Review B, Physical Chemistry Chemical Physics, Surface Science