# Stefan T. Bromley

***Personal Details***


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| 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,<br>c/ Marti i Franques, 1, 08028 Barcelona, Spain<br>Tel. (+34) 93 403 9266, Fax (+34) 93 402 1231<br>E-mail: s.bromley@ub.edu<br>Website: www.ub.edu/nnmgroup |


***Education***

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|---|---|
| 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***

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| 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: 8 (currently supervising 5 PhD students)
Number of Masters theses directed to completion: 5 (currently supervising 2 Masters students)
Total citations: >5400 (ISI Web of Science) / >6500 (Google Scholar)
Av. number of citations per year (last 5 years): 421 (ISI Web of Science) / 538 (Google Scholar)
First and/or corresponding author on >65% of publications
Number of publications: >180 (ISI Web of Science), ~75% of articles in the first quartile, Q1
h-index: 37 (ISI Web of Science) / 40 (Google Scholar)
Book chapters: 8
Books edited: 2
Invited oral presentations: >50
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 5 Master students, 8 PhD students and 4 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 by research line*** (full list at: www.researcherid.com/rid/A-2481-2009)

**IF** = journal impact factor / **COLL** = collaboration with external research group(s).

**Books, special issues & reviews:**

1. **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.

2. **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.

3. **Special Issue:** S. T. Bromley & S. M. Woodley (Eds.) (2016) "Inorganic Nanoclusters: Advances in Understanding Structure and Properties", Inorganics, MDPI. ISSN: 2304-6740.
   - Selected invited papers covering both experimental and theoretical studies of inorganic nanoclusters.

4. **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.

5. **Review:** R. Pfattner, S. T. Bromley, C. Rovira, M. Mas-Torrent (2016) **Tuning Crystal Ordering, Electronic Structure, and Morphology in Organic Semiconductors: Tetrathiafulvalenes as a Model Case**, Adv. Funct. Mater. (Feature article), Adv. Funct. Mater., 26, 2256. **IF**=16.8. **COLL**
   - Review of the properties and progress in tetrathiafulvalene organic semiconductors.

6. **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

7. **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**.
   - Review of methods for modelling inorganic nanoclusters with pertinent case studies.

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

1. 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**=6.9
   - 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-$TiO_2$

2. 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**=6.9 **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.

3. 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.

4. K. C. Ko, S. T. Bromley, J. Y. Lee, F. Illas (2017) **Size-Dependent Level Alignment between Rutile and Anatase $TiO_2$ Nanoparticles: Implications for Photocatalysis**, *J. Phys. Chem. Lett.* 8, 5593. **IF**=7.3 **COLL**.
   - Employing anatase and rutile nanoparticles of different sizes we report a predictive phase diagram of how nanoparticle size affects the anatase-rutile electronic level alignment.

5. S. M. Kozlov, I. Demiroglu, K. M. Neyman, S. T. Bromley, (2015) **Reduced ceria nanofilms from structure prediction**, *Nanoscale* 7, 4361. **IF**=6.9
   - *A new structural phase of reduced ceria with potentially interesting properties is predicted to be viable in epitaxially grown nanofilms.*

*6.* I Demiroglu, S Tosoni, F Illas, ST Bromley (2014) **Bandgap engineering through nanoporosity** *Nanoscale* 6, 1181*.* **IF**=6.9
   - By considering over 100 porous ZnO polymorphs we show how and why nanoporosity can be used to tailor the band gap.

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.

**Astro/nanomineralogy** (Focus on properties of astronomically relevant nanosilicates):

*1.* 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**=5.3
- From quantum chemical calculations we establish a solid basis for arguing that nanosilicates are the likely carriers of the ubiquitous anomalous microwave emission.

2. 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**=3.4 **COLL**
- Based on accurate and intensive global optimization searches we establish the structures and properties of stable Mg-rich olivine and pyroxene nanoclusters.

3. 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**=3.4 **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.

4. D. Gobrecht, I. Cherchneff, A. Sarangi, J. M. C. Plane, S. T. Bromley (2016) **Dust formation in the oxygen-rich AGB star IK Tauri**, *Astronom. Astrophys.* 585, A6. **IF**=5.3 **COLL**
- A highly detailed bottom-up kinetic model of inorganic dust formation around an oxygen-rich evolved star is reported.

5. ST Bromley, JCG Martin, JMC Plane (2016) **Under what conditions does $(SiO)_N$ nucleation occur? A bottom-up kinetic modelling evaluation**, *Phys. Chem. Chem. Phys.* 18, 26913. **IF**=3.4. **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.

*6.* I. Oueslati, B. Kerkeni, S. T. Bromley (2015) **Trends in the Adsorption and Reactivity of Hydrogen on Magnesium Silicate Nanoclusters**, *Phys. Chem. Chem. Phys.* 17, 8951. **IF**=3.4. **COLL**.
- General theoretical exploration into the role of nanosilicates of varying composition in interstellar $H_2$ formation and dissociation.

7. G. Lee, C. Helling, H. Giles, S. T. Bromley (2015) **Dust in Brown Dwarfs and Extra-Solar Planets IV. Assessing $TiO_2$ and SiO Nucleation for Cloud Formation Modelling**, *Astronom. & Astrophys.* 575, A11. **IF**=5.3. **COLL**.
- Theoretical assessment of the respective roles of SiO and $TiO_2$ in cloud formation in brown dwarf-type atmospheres.

8. 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**=5.4. **COLL**.
- Exploration of the interaction of H atoms and molecular hydrogen formation on a nanosilicate with forsterite composition.

9. 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**=5.4. **COLL**.
- First ever detailed atomistic account of how silicate dust could efficiently form around AGB stars.

10. T. P. M. Goumans, S. T. Bromley (2011) **Hydrogen and Oxygen Adsorption on a Nanosilicate – a Quantum Chemical Study**, *Mon. Not. R. Astron. Soc.* 414, 1285. **IF**=5.4. **COLL**.
- *Exploration into the possibility of hydroxylated nanosilicates being the cause of oxygen depletion in interstellar molecular clouds.*

**Organic Electronics/Spintronics** (Focus on materials based on persistent radicals and/or small congugated molecules)**:**

1. 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**=16.8
- We show that out-of-plane compression can tune the correlated electronic states of 2D covalent organic radical materials.

**2.** T. Salzillo, A. Campos, A. Babuji, R. Santiago, S. T. Bromley, C. Ocal, E. Barrena, R. Jouclas, C. Ruzie, G. Schweicher, Y. H. Geerts, M. Mas-Torrent (2020) **Enhancing Long-Term Device Stability Using Thin Film Blends of Small Molecule Semiconductors and Insulating Polymers to Trap Surface-Induced Polymorphs**, *Adv. Funct. Mater.* 30 2006115. **IF**=16.8 **COLL**

- Experiments and theory combine to show that a metastable organic polymorph with technological promise can be stabilised by blending it with an insulating polymer.

3. 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**=7.3 **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.

4. 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**=12.1

- 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.

5. I Alcón, D Reta, I de PR Moreira, ST Bromley (2017) **Design of multi-functional 2D open-shell organic networks with mechanically controllable properties**, *Chem. Sci.* 8, 1027. **IF**=9.3

- We design 2D covalent organic radical farmeworks in which modest in-plane strain is able to tune the electronic properties.

6. 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**=14.6 **COLL**

- An experimental and theoretical study showing how ground state electrons move in anionic molecular wires with radical end-terminations.

7. R. Frisenda, R. Gaudenzi, C. Franco, M. Mas-Torrent, C. Rovira, J. Veciana, I. Alcon, S. T.Bromley, E. Burzurí, H. S. J. van der Zant, (2015) **"Kondo Effect in a Neutral and Stable All Organic Radical Single Molecule Break Junction",** *Nano Lett.*15, 3109. *IF*=11.2 **COLL**

- First ever demonstration of the Kondo effect in a single organic triarylmethyl-derivative radical molecule.

8. F. Grillo, V. Mugnaini, M. Oliveros, S. M. Francis, D-J. Choi, M. V. Rastei, L. Limot, C. Cepek, M. Pedio, S. T. Bromley, N. V. Richardson, J-P. Bucher, J. Veciana (2012) **"Chiral Conformation at a Molecular Level of a Propeller-Like Open-Shell Molecule on Au(111)"** *J. Phys. Chem. Lett.* 3, 1559. *IF*=7.3 **COLL**

- Ordered alternating chiral domains are formed after deposition of triarylmethyl-derivative radicals on the Au(111) surface.

*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**=27.4 **COLL**

- A dramatic change in conductivity is observed and theoretically rationalised in monolayers of two structurally very similar molecules essentially only differing in their electronic structure.

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**=14.6 **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.

***<u>Recent Involvement in Funded Research Projects</u>***

1. **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: €** 4.910.624

2. **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: €** 3.785.868

3. **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: €** 1.082.000

4. **Title:** Unidades de Excelencia María de Maeztu: INSTITUT DE QUIMICA TEORICA I COMPUTACIONAL (IQTC)
   **Principal Investigator:** Francesc Illas (as head of IQTC at time of application)
   **Funding source:** Ministerio de Ciencia e Innovacion, Spain
   **Reference:** MDM-2017-0767
   **Initial/final date:** 2018 / 2022
   **Total awarded**: € 2.000.000

5. **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: €** 164.560

6. **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: €** 38.025

7. **Title:** Modelling Electronic Processes in Nano-Semiconductors: Clusters, Wires and Tubes
   **Principal Investigators:** Stefan Bromley & C. Richard Catlow
   **Funding source:** The Royal Society, UK
   **Reference**: "International Joint Project"
   **Initial/final date:** 2010 / 2012
   **Total awarded: €**16.000

8. **Title:** Ab initio modelling of technologically important materials based on oxides, metals and combinations thereof: from the nanoscale to extended systems.
   **Principal Investigator:** Francesc Illas
   **Funding source:** Ministerio de Ciencia e Innovación, Spain
   **Reference** FIS2008-02238/FIS (Proyecto tipo C, Consolider)
   **Initial/final date:** 2009 / 2013
   **Total awarded: €** 264.000

9. **Title:** Organo-silica interactions relevant to nano/bio-technologies
   **Principal Investigators:** Stefan Bromley & Mariona Sodupe
   **Funding source:** Generalitat de Catalunya, Spain
   **Reference: "**Proyecto de Colaboracion de la Xarxa de Referència de Quimica Teorica i Computacional"
   **Initial/final date:** 2007 / 2008
   **Total awarded: €**30.000

***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).

***<u>Selected oral presentations (>70 given during full career)</u>***

**1. Invited:** “How hot are clusters in experiment? Insights from modelling finite temperature IR spectra”, Symposium on Size Selected Clusters – S3C, Davos (Switzerland, 2020).
**2. Invited:** “Using atomistically detailed simulations to understand the formation, structure and composition of astrophysical silicate dust grains”, IAU Symposium 350 Laboratory Astrophysics: from Observations to Interpretation, Cambridge (UK, 2019).
**3. 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).
**4. Invited: “**Post-graphene organic Dirac materials with tunable spin-polarised and closed-shell semiconducting states”, Graphene Week 2018, San Sebastian, (Spain, 2018).
**5. Invited:** “Structure and Reactivity of Interstellar Nanodust”, European Conference on Surface Science - ECOSS 34, Aarhus (Denmark, 2018).
**6. Invited:** “Tracking the Properties of Oxide Materials from Nanoscale to Bulk”, Multi-Scale Modelling Track, IEEE Nano, Cork (Ireland, 2018).
**7. Invited:** “Learning how Oxide Materials Evolve from Nano to Bulk”, CECAM Workshop: "Big-Data driven Materials Science”, Laussane (Switzerland, 2017).
**8. Invited:** “Silicate dust: a bottom-up computational approach”, Nanocosmos Interstellar Dust Meeting, Toulouse (France, 2017).
**9. 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).
**10. Invited:** “Design of open-shell 2D covalent materials with controllable properties”, European Materials Research Symposium (E-MRS) 2016 Spring Meeting, Lille (France, 2016).
**11 Invited:** “Metal Oxides and their Alloys: Clusters vs Bulk”, Gordon Research Conference on Clusters and Nanostructures, Girona (Spain, 2015).
**12. Keynote:** “Nanocrystals versus Nanoclusters, Limits on Crystallinity and Small Size”, British Association of Crystal Growth Meeting, London (UK, 2015)
**13. Invited:** "Bandgap Engineering via Nanoporosity”, European Materials Research Society (EMRS) Fall Meeting, Warsaw (Poland, 2014).
**14. Invited:** ‘‘A bottom-up computational modelling approach to the formation and properties silicate dust”, 7$^{th}$ meeting on Cosmic Dust, Osaka (Japan, 2014)
**15. Invited lecture series:** “Understanding Cosmic Dust using Computer Modelling” at the “LASSIE” ITN Summer School: “State-of-the-art Astrochemistry”, Paris (France, 2013).
**16. Invited:** “Nucleation of Nanosilicate Clusters: from the Interstellar Medium to Aqueous Solution”, Theory of Atomic and Molecular Clusters VII, Birmingham (UK, 2013).
**17**. **Keynote:** “Nanoscale Ceria: What Can Computational Modelling Tell Us?”, World Resources Forum, National Conference Center, Beijing, (China, 2012).
**18. Invited:** “Structure and properties of nano-oxides: a theoretical overview”, SPIE OPTO Oxide-based Materials and Devices III, Moscone Center, San Francisco, (USA, 2012).
**19. Plenary:** “Unexpected Structural Diversity and New Functional Materials: an Ab Initio Approach”, XXVI Meeting of the Reference Network on Theoretical and Computational Chemistry of Catalonia, (Spain, 2010).
**20. Invited:** On the Persistence of Cluster Stability upon Coalescence into Nanostructures and New Materials”, 4th Jekyll Island International Conference on Clusters and Nanostructures, Georgia (USA, 2010).

***<u>Participation in advisory/examination panels</u>***

**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***

**01/03/2003 - 01/09/2004**: secured 60.000 Euros project funding from Shell Chemicals (Amsterdam, NL) for modelling project: “Understanding Double Metal Catalysts for Propoxylation”.

**01/01/1999 - 31/12/1999**: 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. 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. Piero Ugliengo, University of Turin, Italy
Prof. Thomas Henning, Max Planck Institute for Astronomy, Germany
Dr. Cornelia Jaeger, University of Jena, Germany
Dr. Sandra Lang, Ulm University, Germany
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