Dr. Jordi Poater's CV

Dr. Jordi Poater

City/Date of birth: Banyoles (Girona), Spain/April 21st 1977
Nationality: Spain
Marital status: Married with two daughters
E-mail: jordi.poater@ub.edu
Cell-phone: +34 629756913
Web page: https://www.icrea.cat/Web/ScientificStaff/jordi-poater-teixidor-219355
ResearchID: http://www.researcherid.com/rid/B-5028-2009

Research experience

-ICREA Research Professor (December 2015 – present), Departament de Química Inorgància i Orgànica & Institut de Química Teòrica i Computacional (IQCTUB), Universitat de Barcelona, Barcelona, Spain & Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain.

-Senior associate researcher (February 2014 – November 2016), Department of Theoretical Chemistry, Vrije Universiteit Amsterdam, The Netherlands.

-Research collaborator (April 2014 – April 2015), Wacker Chemie AG, Munich, Germany.

-Postdoc researcher (January 2013 – January 2014), Institute of Computational Chemistry and Department of Chemistry, University of Girona, Girona, Spain.

-***Travel grant Generalitat de Catalunya*** (February-May 2013), Laboratoire de Chimie de Coordination, CNRS, Toulouse, France. Collaboration research visit to Dr. Christine Lepetit and Prof. D. Remi Chauvin.

-***EMBO short-term fellowship*** (September-December 2013), Department of Theoretical Chemistry, Vrije Universiteit Amsterdam, The Netherlands. Collaboration research visit to Prof. Dr. F. Matthias Bickelhaupt and Dr. Célia Fonseca Guerra.

-Ramón y Cajal researcher (January 2008 – December 2012), Institute of Computational Chemistry and Department of Chemistry, University of Girona, Girona, Spain.

-***Travel grant HPC-Europa2 Program*** (October-November 2012), Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands. Collaboration research visit to Prof. Dr. F. Matthias Bickelhaupt.

-***Postdoc researcher / Marie Curie Intra-European Fellowship*** (January 2006 – December 2007), Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands.

-***Postdoc researcher / Travel grant BE from the Generalitat de Catalunya*** (October 2004 – December 2005), Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands.

-***Assistant professor of Physical Chemistry at the University of Girona*** (January 2004 – September 2004), Institute of Computational Chemistry and Department of Chemistry, University of Girona, Girona, Spain.

-***Philosophical Degree in Chemistry*** (January 2000 - December 2003), Institute of Computational Chemistry and Department of Chemistry, University of Girona, Girona, Spain (Predoctoral fellowship for researchers' formation FI from the Generalitat de Catalunya).

PhD thesis (28/04/2003): *"Localization and delocalization indices derived from the bielectronic density: Analysis and applications in molecular structure, chemical reactivity and aromaticity"*, supervised by Prof. Dr. Miquel Solà and Prof. Dr. Miquel Duran.

-***Advanced Studies Diploma in Theoretical and Computational Chemistry*** (22/06/2001), Institute of Computational Chemistry, and Department of Chemistry, University of Girona, Girona, Spain.

-***Travel grant FI from the Generalitat de Catalunya*** (October 2001 – December 2001), Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands. Supervised by Prof. Dr. Evert Jan Baerends.

-***Travel grant FI from the Generalitat de Catalunya*** (October 2002 – December 2002), Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands. Supervised by Prof. Dr. Evert Jan Baerends.

-***Travel grant FI from the Generalitat de Catalunya*** (October 2003 – December 2003), Afdeling Theoretische Chemie, Scheikundig Laboratorium der Vrije Universiteit, Amsterdam, The Netherlands. Supervised by Prof. Dr. Evert Jan Baerends.

-***Collaboration fellowship University / Pharmaceutical Company: Medichem S.A.*** (July 1999 – December 1999), University of Girona, Girona, Spain.

-***Bachelor of Science Degree in Chemistry*** (September 1995 - July 1999), University of Girona, Girona, Spain.

-Collaboration fellowship for researchers' formation from the Spanish Education and Science Ministry (September 1998 – June 1999), Institute of Computational Chemistry, University of Girona, Girona, Spain.

Participation in R+D Projects

- "*Design of new materials with specific nonlinear optical properties. New methodological developments for the correct prediction of the interactions and vibrational contributions*" (PB98-0457-C02-01, Spanish Science and Technology Ministry), Prof. Dr. Miquel Duran, Institute of Computational Chemistry, University of Girona (1999-2002).
- "*Development of new reactivity indices based in the conceptual Density Functional Theory for the theoretical study of the chemical reactivity*" (Generalitat de Catalunya), Prof. Dr. Miquel Solà, Institute of Computational Chemistry, University of Girona (2001-2003).
- "*The retro-Bingel reaction as a strategy for the selective functionalization of fullerenes: Theoretical study of the reaction mechanism*" (University of Girona), Prof. Dr. Miquel Solà, Institute of Computational Chemistry, University of Girona (2001-2002).
- "*Structure and reactivity of Fischer carbenes*" (Generalitat de Catalunya), Prof. Dr. Miquel Solà, Institute of Computational Chemistry, University of Girona (2001-2004).
- "*Ionization and activation through methylic cations of biochemical systems. Theoretical studies of mass spectroscopy*" (BQU2002-04112-C02-02, Spanish Science and Technology Ministry), Prof. Dr. Miquel Solà, Institute of Computational Chemistry, University of Girona (2002-2005).
- "*Development and application of ab initio methodology to the engineering of molecular crystals and functionalised polymers which exhibit high nonlinear optical properties*" (BQU2003-03334, Spanish Science and Technology Ministry), Prof. Dr. Miquel Duran, Institute of Computational Chemistry, University of Girona (2002-2005).
- "*Structure and reactivity – Theory-bases design*" (VICI Award, Netherlands organization of scientific research – NOW), Prof. Dr. F. Matthias Bickelhaupt, Theoretical Chemistry Department, Vrije Universiteit Amsterdam (2002-2006).
- "*Molecular recognition and template directed synthesis: Electronic, steric and solvent effects in biocatalytic DNA replication*" (National research school combination-catalysis – NRSCC), Prof. Dr. F. Matthias Bickelhaupt, Theoretical Chemistry Department, Vrije Universiteit Amsterdam (2005-2009).
- "*DNA replication and biomolecular recognition*" (IEF Marie Curie, European Commission), Dr. **Jordi Poater**, Theoretical Chemistry Department, Vrije Universiteit Amsterdam (2006-2007), 167.000€.
- "*Activation of biomolecules. Computational and mass spectrometry studies*" (CTQ2005-08798-C02-01/BQU, Spanish Education and Science Ministry), Co-Investigator, PI: Prof. Dr. Miquel Solà, Institute of Computational Chemistry, University of Girona (2005-2008).
- "*Quantum biochemistry: DNA replication and biomolecular recognition*" (Ramón y Cajal, Spanish Education and Science Ministry), PI: Dr. **Jordi Poater**, Institute of Computational Chemistry, University of Girona (2008-2012), 189.000 €.

- "*Quantumbiology: DNA replication and biomolecular recognition*" (European Reintegration Grant, European Commission), PI: Dr. **Jordi Poater**, Institute of Computational Chemistry, University of Girona (2009-2012), 45000 €.
- "*Reactivity and chemical bonding in biomedicine and (bio)inorganic chemistry*" (CTQ2008-06532/BQU, Spanish Education and Science Ministry), Co-Investigator, PI: Dr. Marcel Swart, ICREA and Institute of Computational Chemistry, University of Girona (2009-2011).
- "*Metallic and semimetallic clusters. Aromaticity and reactivity studies*" (CTQ2008-03077/BQU, Spanish Science and Innovation Ministry), Co-Investigator, PI: Prof. Dr. Miquel Solà, Institute of Computational Chemistry, University of Girona (2009-2011).
- "*Theoretical Chemistry and Molecular Modelling and Engineering*" (SGR2009-528), Generalitat de Catalunya, Co-Investigator, PI: Dr. Lluís Blancafort, Institute of Computational Chemistry, University of Girona (2009-2011).
- "*DNA replication: Estimating the effects and interplay of solvation, pi-stacking, hydrogen bonding and selectivity*" (QCM-2009-1-0018, QCM-2009-2-0008, QCM-2009-3-0015, Marenostrum Spanish Supercomputing Net, 670.000 hours), PI: Dr. **Jordi Poater**, Institute of Computational Chemistry, University of Girona (2009).
- "*Multiscalar modelization in (bio)chemistry*" (CTQ2011-25086), Spanish Science and Innovation Ministry), Co-Investigator, PI: Dr. Marcel Swart, ICREA and Institute of Computational Chemistry, University of Girona (2012-2014).
- "How do (exo)planetary environments affect chemistry & spectra of (supposed) biomarkers and geochemical processes?" (NWO-648.001.003), Netherlands Organisation for Scientific Research, Co-PI: **Jordi Poater**, Vrije Universiteit Amsterdam, The Netherlands (2014-2017), 226.121 EUR.
- "Silicon alpha-effecct: a systematic experimental and computational study of the hydrolysis of functionalized alkoxytriorganylsilanes", PI: **Jordi Poater**, Wacker Chemie AG, Vrije Universiteit Amsterdam, The Netherlands (2014-2015), 55.000 EUR.
- "Diseño computacional de pares de bases de ADN artificiales que pueden ser replicados" (CTQ2016-77558-R), Ministerio de Economía y Competitividad (MINECO), PI: **Jordi Poater**, Universitat de Barcelona, Spain (2016-2019), 36.300 EUR.
- "Palladium-catalyzed oxidative aerobic isocyanide insertion. A mechanistic study", Holland Research School of Molecular Chemistry (2016), 10.500 EUR.
- "Modelització i disseny de sistemes químics radicalaris" (2017SGR348), PI: Josep Maria Bofill, Researcher: Jordi Poater, Universitat de Barcelona, Spain (2017-2019), 20.000 EUR.
- "Organization of the Annual meeting of the Reference Network of Theoretical and Computational Chemistry of Catalonia – XRQTC", Societat Catalana de Química, PI: Jordi Poater, Universitat de Barcelona, Spain (2018), 500 EUR.
- "Centros de Excelencia Severo Ochoa y Unidades de Excelencia María de Maeztu", Ministerio de Economía y Competitividad (MINECO), co-PI: **Jordi Poater**, Universitat de Barcelona, Spain (2018-2022), 2.000.000 EUR.
- Ayudas para contratos predoctorales para la formación de doctores, Ministerio de Ciencia, Innovación y Universidades, student: David Almacellas, PI: **Jordi Poater**, Universitat de Barcelona, Spain (2019-2023), 120.000 EUR.
- "Modelling non-covalent interactions and cooperativity in (un)natural DNA base pairs and guanine quadruplexes", Ministerio de Ciencia, Innovación y Universidades, PI: **Jordi Poater**, Universitat de Barcelona, Spain (2020-2023), 60.500 EUR.
- "Laboratori de Materials Inorgànics i Catàlisi / LMI" (2021SGR442), Generalitat de Catalunya, PI: Rosario Núñez, Researcher: **Jordi Poater**, Universitat de Barcelona, Spain (2020-2023), 40.000 EUR.
- "Centros de Excelencia Severo Ochoa y Unidades de Excelencia María de Maeztu" (CEX2021-001202-M), Ministerio de Ciencia, Innovación y Universidades, PI: Eliseo Ruiz, Researcher: **Jordi Poater**, Universitat de Barcelona, Spain (2023-2027), 2.000.000 EUR.
- "Interacciones no-covalentes en macromoléculas de ADN no-naturales y clústeres de boro" (PID2022-138861NB-I00), Ministerio de Ciencia, Innovación y Universidades, PI: **Jordi Poater**, Universitat de Barcelona, Spain (2022-2025), 125.000 EUR.

- Programa de contractació d'investigadors predoctorals de la Universitat de Barcelona, Universitat de Barcelona, student: Sergi Betkohshvili, PI: **Jordi Poater**, Universitat de Barcelona, Spain (2024-2026), 100.000 EUR.
- FI-SDUR 2023 PhD: "Ajuts de suport a departamnets i unitats de recerca universitaris per a la contractació de personal investigador predoctoral en formación", Generalitat de Catalunya, student: Sergi Betkohshvili, PI: **Jordi Poater**, Universitat de Barcelona, Spain (2024-2026), 100.000 EUR.

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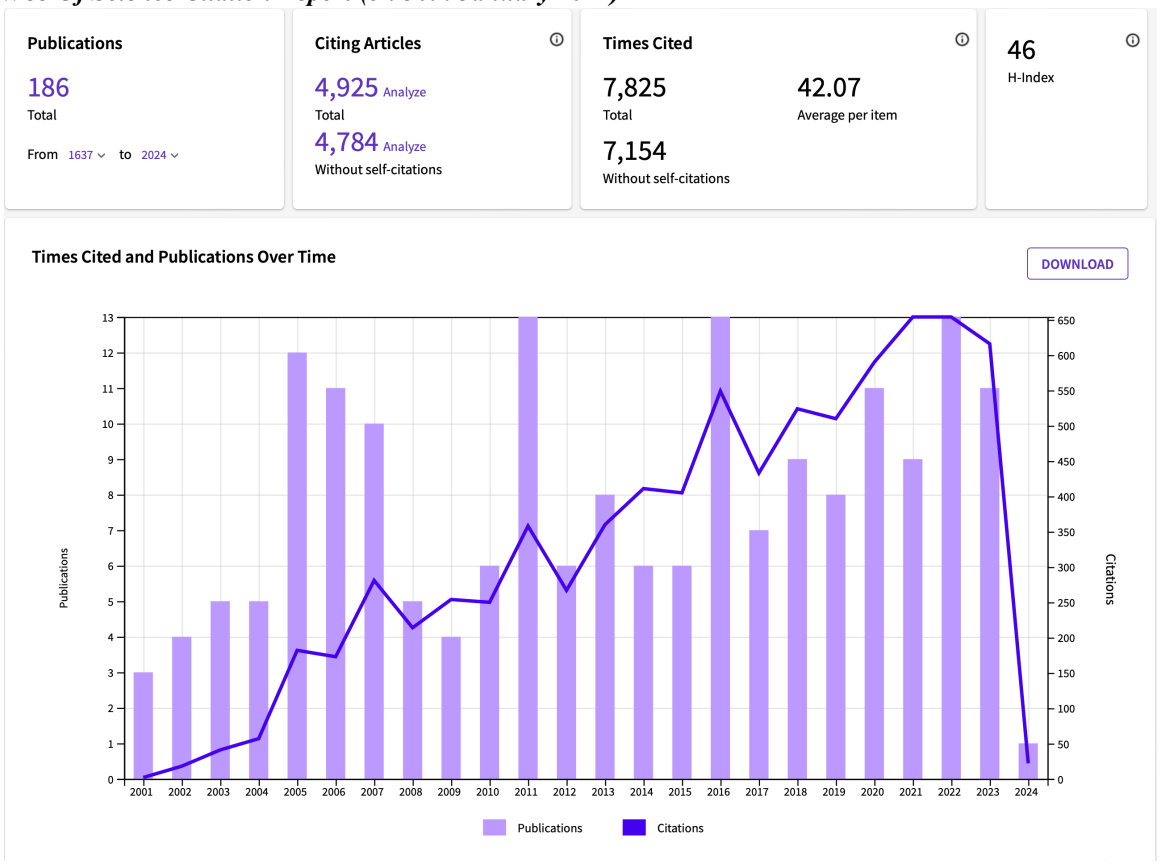

Publications

1. "*New insights in chemical reactivity by means of electron pairing analysis*".
   Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera
   Journal of Physical Chemistry A **2001**, *105*, 2052-2063.
   Journal of Physical Chemistry A **2002**, *106*, 4794 *(Erratum)*.
2. "*Effects of solvation on the pairing of electrons in a series of simple molecules and in the Menshutkin reaction*".
   Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera
   Journal of Physical Chemistry A **2001**, *105*, 6249-6257.
3. "*Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques*".
   Jordi Poater, Miquel Duran, and Miquel Solà
   Journal of Computational Chemistry **2001**, *22*, 1666-1678.
4. "*Analysis of the effect of changing the a_0 parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions*".
   Jordi Poater, Miquel Solà, Miquel Duran, and Juvencio Robles

Physical Chemistry Chemical Physics **2002**, *4*, 722-731.

5. "*The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory*".
   Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera
   Theoretical Chemistry Accounts **2002**, *107*, 362-371.
6. "*Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory*".
   Xavier Fradera, Jordi Poater, Sílvia Simon, Miquel Duran, and Miquel Solà
   Theoretical Chemistry Accounts **2002**, *108*, 214-224.
7. "*Bielectronic densities: Analysis and applications in molecular structure and chemical reactivity*".
   Jordi Poater, Miquel Solà, Miquel Duran, Juvencio Robles, and Xavier Fradera
   "***Reviews of modern quantum chemistry. A celebration of the contributions of Robert G. Parr***", edited by K. D. Sen, World Scientific, Singapur, **2002**, pp. 831-870.
8. "*The local aromaticities in buckybowls. From planar polycyclic aromatic hydrocarbons to C_{60}*".
   Jordi Poater, Xavier Fradera, Miquel Duran, and Miquel Solà
   "***Fullerenes: The exciting world of nanocages and nanotubes***", edited by P. V. Kamat, K. M. Kadish and D. Guldi, The Electrochemical Society Inc., Pennington, Vol. 12, **2002**, pp. 707-719.
9. "*The delocalization index as an electronic aromaticity criterion: Application to a series of planar polycyclic aromatic hydrocarbons*".
   Jordi Poater, Xavier Fradera, Miquel Duran, and Miquel Solà
   Chemistry A European Journal **2003**, *9*, 400-406.
10. "*An insight into the local aromaticities of polycyclic aromatic hydrocarbons and fullerenes*".
    Jordi Poater, Xavier Fradera, Miquel Duran, and Miquel Solà
    Chemistry A European Journal **2003**, *9*, 1113-1122.
11. "*On the electron-pair nature of the hydrogen bond in the framework of the atoms in molecules theory*".
    Jordi Poater, Xavier Fradera, Miquel Solà, Miquel Duran, and Sílvia Simon
    Chemical Physics Letters **2003**, *369*, 248-255.
12. "*Nuclear magnetic resonance (NMR) chemical shifts with the statistical average of orbital-dependent model potentials (SAOP) in Kohn-Sham DFT*".
    Jordi Poater, Erik van Lenthe, and Evert Jan Baerends
    Journal of Chemical Physics **2003**, 118, 8584-8593.
13. "*Electron pairing analysis of the Fischer-type chromium-carbene complexes $(CO)_5Cr=C(X)R$ (X = H, OH, OCH_3, NH_2, $NHCH_3$ and R = H, CH_3, $CH=CH_2$, Ph, $C\equiv CH$)*".
    Jordi Poater, Montserrat Cases, Xavier Fradera, Miquel Duran, and Miquel Solà
    Chemical Physics **2003**, 294, 129-139.
14. "*An analysis of electronic delocalization in Buckminsterfullerene (C_{60})*".
    Jordi Poater, Miquel Duran, and Miquel Solà
    International Journal of Quantum Chemistry **2004**, 98, 361-366.
15. "*Discrepancy between common local aromaticity measures in a series of carbazole derivatives*".
    Jordi Poater, Isidoro García-Cruz, Francesc Illas, and Miquel Solà
    Physical Chemistry Chemical Physics **2004**, 6, 314-318.
16. "*Grown and low-lying states of Cu^{2+}-H_2O. A difficult case for density functionals methods* ".
    Jordi Poater, Miquel Solà, Albert Rimola, Luís Rodríguez-Santiago, and Mariona Sodupe
    Journal of Physical Chemistry A **2004**, 108, 6072-6078.
17. "*Relation between the substituent effect and aromaticity* ".
    Tadeusz M. Krygowski, Krzysztof Ejsmont, Beata T. Stepien, Michal K. Cyranski, Jordi Poater, and Miquel Solà
    Journal of Organic Chemistry **2004**, *69*, 6634-6640.
18. "*Local aromaticity of the six-membered rings in pyracylene. A difficult case for the NICS indicator or aromaticity*".
    Jordi Poater, Miquel Solà, Rosario G. Viglione, and Roberto Zanasi
    Journal of Organic Chemistry **2004**, 69, 7537-7542.
19. "*Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride*".

Anbarasan Kalaiselvan, Ponnambalam Venuvanalingam, Jordi Poater, and Miquel Solà
International Journal of Quantum Chemistry **2005**, *102*, 139-146.

20. "*Hydrogen bonding and aromaticity in the guanine-cytosine base pair interacting with metal cations (M = Cu^{+}, Ca^{2+} and Cu^{2+})*".
Jordi Poater, Mariona Sodupe, Joan Bertran, and Miquel Solà
Molecular Physics **2005**, *103*, 163-173.
21. "*Comment on Nature of bonding in the thermal cyclization of (Z)-1,2,4,6-heptatetraene and its heterosubstituted analogues*".
Eduard Matito, Miquel Solà, Miquel Duran, and Jordi Poater
Journal of Physical Chemistry B **2005**, *109*, 7591-7593.
22. "*An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Diels-Alder reaction. Exploring the validity of different indicators of aromaticity*".
Eduard Matito, Jordi Poater, Miquel Duran, and Miquel Solà
Journal of Molecular Structure (THEOCHEM) **2005**, *727*, 165-171.
23. "*Local aromaticity of [n]acenes, [n]phenacenes, and [n]helicenes (n = 1-9)*".
Guillem Portella, Jordi Poater, Josep M. Bofill, Pere Alemany, and Miquel Solà
Journal of Organic Chemistry **2005**, *70*, 2509-2521.
24. "*Theoretical evaluation of electron delocalization in aromatic molecules by means of AIM and ELF topological approaches*".
Jordi Poater, Miquel Duran, Miquel Solà, and Bernard Silvi
Chemical Reviews **2005**, *105*, 3911-3947.
25. "*Diastereoselective synthesis of fulleropyrrolidines from suitably functionalized chiral cyclobutanes*".
Beatriz M. Illescas, Nazario Martín, Jordi Poater, Miquel Solà, Gemma P. Aguado, and Rosa M. Ortuño
Journal of Organic Chemistry **2005**, *70*, 6929-6932.
26. "*An aromaticity analysis of lithium-cation/pi complexes of aromatic systems*".
Mireia Güell, Jordi Poater, Josep M. Luis, Otilia Mó, Manuel Yáñez, and Miquel Solà
ChemPhysChem **2005**, *6*, 2552-2561.
27. "*Comparison of the AIM delocalization index and the Mayer and fuzzy atom bond orders*".
Eduard Matito, Jordi Poater, Miquel Solà, Miquel Duran, and Pedro Salvador
Journal of Physical Chemistry A **2005**, *109*, 9904-9910.
28. "*Local aromaticity of the lowest-lying singlet states of [n]acenes (n = 6-9)*".
Jordi Poater, Josep M. Bofill, Pere Alemany, and Miquel Solà
Journal of Physical Chemistry A **2005**, *109*, 10629-10632.
29. "*Assessment of the Clar's aromatic pi-sextet rule by means of PDI, NICS, and HOMA indicators of aromaticity*".
Guillem Portella, Jordi Poater, and Miquel Solà
Journal of Physical Organic Chemistry **2005**, *18*, 785-791.
30. "*Electron fluctuation in pericyclic and pseudopericyclic reactions*".
Eduard Matito, Jordi Poater, Miquel Duran, and Miquel Solà
ChemPhysChem **2006**, *7*, 111-113.
31. "*Role of electron density and magnetic couplings on the nucleus-independent chemical shift (NICS) profiles of [2.2]paracyclophane and related species*".
Jordi Poater, Josep M. Bofill, Pere Alemany, and Miquel Solà
Journal of Organic Chemistry **2006**, *71*, 1700-1702.
32. "*Hydrogen-hydrogen bonding in planar biphenyl, predicted by Atoms-in-Molecules, does not exist*".
Jordi Poater, Miquel Solà and F. Matthias Bickelhaupt
Chemistry A European Journal **2006**, *12*, 2889-2895.
33. "*A trinuclear Pt(II) compound with short Pt-Pt contacts. An analysis of the influence of pi-stacking interaction on the strength and length of the Pt-Pt bond*".
Albert Poater, Silvia Moradell, Eduard Pinilla, Jordi Poater, Miquel Solà, Antoni Llobet, M. Angeles Martinez
Dalton Transactions **2006**, *109*, 1188-1196.

34. "*Bonding in methylalkalimetals $(CH_3M)_n$ (M = Li, Na, K; n = 1, 4). Agreement and divergences between AIM and ELF analyses*".
Eduard Matito, Jordi Poater, F. Matthias Bickelhaupt, and Miquel Solà
Journal of Physical Chemistry B **2006**, *110*, 7189-7198.
35. "*A model of the chemical bond must be rooted in quantum mechanics, provide insight, and possess predictive power*".
Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt
Chemistry A European Journal **2006**, *12*, 2902-2905.
36. "*Analysis of electron delocalization in aromatic systems: individual molecular orbital contributions to para-delocalization indexes (PDI)*".
Mireia Güell, Eduard Matito, Josep M. Luis, Jordi Poater, and Miquel Solà
Journal of Physical Chemistry A **2006**, *110*, 11569-11574.
37. "*Are nucleus-independent (NICS) and 1H-NMR chemical shifts good indicators or aromaticity in pi-stacked polyfluorenes?*".
Sílvia Osuna, Jordi Poater, Josep M. Bofill, Pere Alemany, and Miquel Solà
Chemical Physics Letters **2006**, *428*, 191-195.
38. "*Cuestionada la interpretación de Bader sobre el significado de los puntos críticos de enlace*".
Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt
Anales de la RSEQ **2006**, *102*, 36-36.
39. "*Local aromaticity in natural nucleobases and their size-expanded benzo-fused derivatives*".
Oscar Huertas, Jordi Poater, M. Fuentes-Cabrera, Modesto Orozco, Miquel Solà, and F. Javier Luque
Journal of Physical Chemistry A **2006**, *110*, 12249-12258.
40. "*Electronic structure and reactivity of aromatic metal clusters*".
P. Gonzalez, Jordi Poater, Gabriel Merino, T. Heine, Miquel Solà, and Juvencio Robles
"***Theoretical aspects of chemical reactivity. Theoretical and computational chemistry series***", edited by A. Toro-Labbé, ElSevier, Amsterdam, **2007**, vol. 19, pp. 203-218.
41. "*Aromaticity analyses by means of the quantum theory of atoms in molecules*".
Eduard Matito, Jordi Poater, and Miquel Solà
"***The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design***", edited by C. F. Matta and R. J. Boyd, Wiley-VCH, New York, **2007**, pp. 399-423.
42. "*Polycyclic benzenoids. Why kinded is more stable than straight*".
Jordi Poater, Ruud Visser, Miquel Solà, and F. Matthias Bickelhaupt
Journal of Organic Chemistry **2007**, *72*, 1134-1142.
43. "*Is the aromaticity of the benzene ring in the (eta6-C_6H_6)$CrCO_3$ complex larger than that of the isolated benzene molecule?*".
Ferran Feixas, J. Oscar C. Jiménez-Halla, Eduard Matito, Jordi Poater, and Miquel Solà
Polish Journal of Chemistry **2007**, *81*, 783-797.
44. "*Aromaticity of distorted benzene rings: Exploring the validity of different indicators of aromaticity*".
Ferran Feixas, Eduard Matito, Jordi Poater, and Miquel Solà
Journal of Physical Chemistry A **2007**, *111*, 4513-4521.
45. "*Didehydrophenanthrenes: Structure, singlet-triplet splitting, and aromaticity*".
Jordi Poater, F. Matthias Bickelhaupt, and Miquel Solà
Journal of Physical Chemistry A **2007**, *111*, 5063-5070.
46. "*New solids based on B12N12 fullerenes*".
Jon M. Matxain, Leif A. Eriksson, Jose M. Mercero, Xabier Lopez, M. Piris, Jesus M. Ugalde, Jordi Poater, Eduard Matito, and Miquel Solà
Journal of Physical Chemistry C **2007**, *111*, 13354-13360.
47. "Aromaticity changes along the reaction coordinate connecting the cyclobutane dimer to cubane and the benzene dimer to hexaprismane".
Mercedes Alonso, Jordi Poater, and Miquel Solà
Structural Chemistry **2007**, *18*, 773-783.
48. "*On the performance of some aromaticity indices: A critical assessment using a test set*".

Ferran Feixas, Eduard Matito, Jordi Poater, and Miquel Solà
Journal of Computational Chemistry **2008**, *29*, 1543-1554.

49. "*Hypervalent versus nonhypervalent carbon in noble-gas complexes*".
Simon C. A. H. Pierrefixe, Jordi Poater, Chan Im, and F. Matthias Bickelhaupt
Chemistry A European Journal **2008**, *14*, 6901-6911.

50. "*Biphenyls, bond paths and repulsions: Do the ortho and ortho' substituents in biphenyls repel attract (bind to) each other?*".
Jordi Poater, Joseph J. Dannenberg, Miquel Solà, and F. Matthias Bickelhaupt
International Journal of Chemical Modeling **2008**, *1*, 63-78.

51. "*Analysis of Hückel's [4n+2] rule through electronic delocalization measures*".
Ferran Feixas, Eduard Matito, Miquel Solà, and Jordi Poater
Journal of Physical Chemistry A **2008**, *112*, 13231-13238.

52. "*Aromaticity and chemical reactivity*".
Eduard Matito, Jordi Poater, Miquel Solà, and Paul v. R. Schleyer
"Chemical Reactivity Theory", edited by P. K. Chattaraj, Taylor & Francis/CRC Press, Boca Ratón, **2009**, pp. 419-438.

53. "*Alkali metal complexes of silyl-substituted ansa-(tris)allyl ligands: Metal-, co-ligand- and substituent dependent stereochemistry*".
Scott A. Sulway, Roman Girshfeld, Sophia A. Solomon, Christopher A. Muryn, Jordi Poater, Miquel Solà, F. Matthias Bickelhaupt, and Richard A. Layfield
European Journal of Inorganic Chemistry **2009**, 4157-4167.

54. "*Modeling the structure-property relationship of nanoneedles: A journey toward nanomedicine*".
Albert Poater, Ana Gallegos, Ramon Carbó-Dorca, Jordi Poater, Miquel Solà, Luigi Cavallo, and A. P. Worth
Journal of Computational Chemistry **2009**, *30*, 275-284.

55. "*Excess charge delocalization in organic and biological molecules: some theoretical notions*".
Lluís Blancafort, Miquel Duran, Jordi Poater, Pedro Salvador, Sílvia Simon, Miquel Solà, and Alexander Voityuk
Theoretical Chemistry Accounts **2009**, *123*, 29-40.

56. "*Twisted phenanthrene and other molecular victims of steric repulsion*".
Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt
International Journal of Chemical Modeling **2010**, *2*, 181-194.

57. "*Examining the planarity of poly(3,4-ethylenedioxythiophene): Consideration of self-rigidification, electronic, and geometric effects*".
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Thomas Hansen, Xiaobo Sun, Marco Dalla Tiezza, Willem-Jan Van Zeist, Jordi Poater, Trevor A. Hamlin, F. Matthias Bickelhaupt

Chemistry A European Journal 2022, 28, e202103953. DOI: 10.1002/chem.202103953.

149.-"Aromaticity and Extrusion of Benzenoids Linked to [o-COSAN]-. Clar has the Answer".

Jordi Poater, Clara Viñas, David Olid, Miquel Solà, Francesc Teixidor

Angewandte Chemie International Edition 2022, 61, e202200672. DOI: 10.1002/anie.202200672. HOT PAPER

150.-"Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins".

Roman Belle, Jos J. A. G. Kamps, Jordi Poater, Kiran Kumar, Bas J. G. E. Pieters, Eidarus Salah, Timothy D. W. Claridge, Robert S. Paton, F. Matthias Bickelhaupt, Akane Kawamura, Christopher J. Schofield, Jasmin Mecinović

Communications Chemistry 2022, 5, 27. DOI: 10.1038/s42004-022-00640-4.

151.-"Probing Noncovalent Interactions in [3,3]Metaparacyclophanes".

Jie Jian, Roel Hammink, Paul Tinnemans, F. Matthias Bickelhaupt, Christine J. McKenzie, Jordi Poater, Jasmin Mecinović

Journal of Organic Chemistry 2022, 87, 6087-6096. DOI: 10.1021/acs.joc.2c00350.

152.-"C-X Bond Activation by Palladium: Steric Shielding versus Steric Attraction".

Thomas Hansen, Xiaobo Sun, Marco Dalla Tiezza, Willem-jan van Zeist, Joost N. P. van Stralen, Daan P. Geerke, Lando P. Wolters, Jordi Poater, Trevor A. Hamlin, F. Matthias Bickelhaupt

Chemistry A European Journal 2022, 28, e202201093. DOI: 10.1002/chem.202201093.

153.-"Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings".

Jie Jian, Darina Barkhatova, Roel Hammink, Paul Tinnemans, F. Matthias Bickelhaupt, Jordi Poater, Jasmin Mecinović

Journal of Organic Chemistry 2022, 87, 7875-7883. DOI: 10.1021/acs.joc.2c00533.

154.-"3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives".

Jordi Poater, Clara Viñas, Miquel Solà, Francesc Teixidor

Nature Communications 2022, 13, 3844. DOI: 10.1038/s41467-022-31267-7.

155.-"Ni(i)-TPA stabilization by hydrogen bond formation on the second coordination sphere: a DFT characterization".

Sergio Posada-Pérez, Sílvia Escayola, Jordi Poater, Miquel Solà, Albert Poater

Dalton Transactions 2022, 51, 12585-12595. DOI: 10.1039/d2dt01355j.

156.-“Unravelling Enzymatic Features in a Supramolecular Iridium Catalyst by Computational Calculations”.

Michele Tomasini, Lucia Caporaso, Jonathan Trouve, Jordi Poater, Rafael Gramage-Doria, Albert Poater

Chemistry A European Journal 2022, 28, e202201970. DOI: 10.1002/anie.202207477.

157.-“Methyl Substitution Destabilizes Alkyl Radicals”.

Eva Blokker, Willem-Jan van Zeist, Xiaobo Sun, Jordi Poater, J. Martijn van der Schuur, Trevor A. Hamlin, F. Matthias Bickelhaupt

Angewandte Chemie International Edition 2022, 61, e202207477. DOI: 10.1038/s41467-022-31267-7.

158.-“Rational design of iron catalysts for C-X bond activation”.

Xiaobo Sun, Thomas Hansen, Jordi Poater, Trevor A. Hamlin, F. Matthias Bickelhaupt

Journal of Computational Chemistry 2023, 44, 495-505. DOI: 10.1002/jcc.26818.

159.-“Facile Construction of New Hybrid Conjugation via Boron Cage Extension”.

Fangxiang Sun, Shuaimin Tan, Hou-Ji Cao, Chang-Sheng Lu, Deshuang Tu, Jordi Poater, Miquel Solà, Hong Yan

Journal of the American Chemical Society 2023, 145, 3577-3587. DOI: 10.1021/jacs.2c12526.

160.-“Metallic-Organic Cages (MOCs) with Heterometallic Character: Flexibility-Enhancing MOFs”.

Sergio Posada-Pérez, Jordi Poater, Naiemeh Bahri-Laleh, Albert Poater

Catalysts 2023, 13, 317. DOI: 10.3390/catal13020317.

161.-“Probing Polar-π Interactions Between Tetrazoles and Aromatic Rings”.

Jie Jian, Roel Hammink, Paul Tinnemans, F. Matthias Bickelhaupt, Jordi Poater, Jasmin Mecinović

Chemistry An Asian Journal 2023, 18, e202300192. DOI: 10.1002/asia.202300192.

162.-“Insertion of CO_2 and CS_2 into Bi-N bonds enables catalyzed CH-activation and light-induced bismuthinidene transfer”.

Kai Oberdorf, Anna Hanft, Xiulan Xie, F. Matthias Bickelhaupt, Jordi Poater, Crispin Lichtenberg

Chemical Science 2023, 14, 5214-5219. DOI: 10.1039/d3sc01635h.

163.-“Controlling the Diradical Character of Thiele Like Compounds”.

Josep M. Anglada, Jordi Poater, Ibeirio de P. R. Moreira, Josep M. Bofill

Journal of Organic Chemistry 2023, 13, 8553–8562. DOI: 10.1021/acs.joc.3c00482.

164.-“On the existence of collective interactions reinforcing the metal-ligand bond in organometallic compounds”.

Jordi Poater, Pascal Vermeeren, Trevor A. Hamlin, F. Matthias Bickelhaupt, Miquel Solà

Nature Communications 2023, 14, 3872. DOI: 10.1038/s41467-023-39498-y.

165-“Pioneering the Power of TwinBonds in a Revolutionary Double Bond Formation. Unveiling the True Identity of o-Carboryne as o-Carborene”.

Jordi Poater, Clara Viñas, Sílvia Escayola, Miquel Solà, Francesc Teixidor

Chemistry A European Journal 2023, 29, e202302448. DOI: 10.1002/chem.202302448. VIP ARTICLE

166.-“Single-Not Double-3D-Aromaticity in an Oxidized *Closo* Icosahedral Dodecaiodo-Dodecaborate Cluster”.

Jordi Poater, Sílvia Escayola, Albert Poater, Francesc Teixidor, Henrik Ottosson, Clara Viñas, Miquel Solà

Journal of the American Chemical Society 2023, 145, 22527-22538. DOI: 10.1021/jacs.3c07335.

167.-“Strengthened cooperativity of DNA-based cyclic hydrogen-bonded rosettes by subtle functionalization”.

David Almacellas, Célia Fonseca Guerra, Jordi Poater

Organic & Biomolecular Chemistry 2023, 21, 8403-8412. DOI: 10.1039/d3ob01391j.

168.-“Non-Innocent π Linkers Affect Cooperativity in Hydrogen-Bonded Macrocycles”.

David Almacellas, Stephanie C. C. van der Lubbe, Alice A. Grosch, Iris Tsagri, Jordi Poater, Célia Fonseca Guerra

ChemistryEurope 2023, e202300036. DOI: 10.1002/ceur.202300036.

169.-"Brownmillerite Calcium Ferrite, a Promising Perovskite-Related Material in the Degradation of a Tight Dye under Ambient Conditions".
Zahra Noori, Azim Malekzadeh, Jordi Poater
ChemistryOpen 2023, e202300169. DOI: 10.1002/open.202300169.

170.-"Multiple hydrogen-bonded dimers: Are only the frontier atoms relevant?".
Celine Nieuwland, David Almacellas, Mac M. Veldhuizen, Lucas de Azevedo Santos, Jordi Poater, Célia Fonseca Guerra
Physical Chemistry Chemical Physics 2023. DOI: 10.1039/D3CP05244C.

171.-"Cooperativity in Hydrogen-Bonded Macrocycles Derived from Nucleobases".
David Almacellas, Stephanie C. C. van der Lubbe, Alice A. Grosch, Iris Tsagri, Célia Fonseca Guerra, Jordi Poater
European Journal of Organic Chemistry 2023, e202301164. DOI: 10.1002/ejoc.202301164.

Participation in scientific events

1. ***Electron Densities and Electron Distributions Workshop.***
   San Sebastian, Spain; April 27-28, 2000.
   -***Poster:*** "*Optimizing hybrid density functionals by means of quantum molecular similarity techniques*", Jordi Poater, Miquel Duran, and Miquel Solà.
2. ***Satellite Symposium of the 10th International Congress of Quantum Chemistry.***
   Menton, France; June 11-14, 2000.
   -***Poster:*** "*Parametrizing the B3LYP hybrid functional using quantum molecular similarity techniques*", Miquel Solà, Miquel Duran, and Jordi Poater.
3. ***Annual meeting of the theoretical chemistry net of the Generalitat de Catalunya.***
   Barcelona, Spain; July 13-15, 2000.
   -***Communication:*** "*Localization and delocalization indices. Application to the chemical reactivity*", Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera.
4. ***European Summerschool in Quantum Chemistry (ESQC-00).***
   Riolo Terme, Italy; September 17-30, 2000.
   -***Poster:*** "*Analysis of electron pairing reorganization in a series of chemical reactions*", Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera.
5. ***International Conference on Electronic Structure: Prediction and Applications.***
   San Sebastian, Spain; October 4-6, 2000.
   -***Poster:*** "*Chemical reactivity and electron pairing: analysis of a series of common reactions*", Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera.
6. ***V Molecular Seminar on Molecular Similarity: Molecular Similarity, Density Functions & Applied Theoretical Chemistry.***
   Girona, Spain; July 12-20, 2001.
   -***Communication:*** "*Are the B3LYP bielectronic indices superior to those obtained with the Hartree-Fock method?*", Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera.
7. ***9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics.***
   Madrid, Spain; September 10-14, 2001.
   -***Poster:*** "*Effect of the variation of the Becke3-LYP parameters on physicochemical properties*", Jordi Poater, Miquel Duran, and Miquel Solà.
8. ***Electronic Structure and Chemical Reactivity. An international Symposium in*** **Honor of Prof. Juan Bertrán.**
   Bellaterra, Spain; September 19-22, 2001.
   -***Poster:*** "*Effects of solvation on the electron pairing analysis*", Jordi Poater, Miquel Solà, Miquel Duran, and Xavier Fradera.
9. ***201st Meeting of the Electrochemical Society (ECS).***
   Philadelphia, United States; May 12-17, 2002.

-***Conference:*** "*The aromaticity in bowl-shaped polycyclic aromatic hydocarbons*", Miquel Solà, Jordi Poater, Miquel Duran, and Xavier Fradera.

10. XVIII meeting of the theoretical and computational chemistry net of Catalonia.

Barcelona, Spain; July 8-10, 2002.

-***Communication:*** "*The delocalization index as a new electronic aromaticity criterion*", Jordi Poater, Xavier Fradera, Miquel Duran, and Miquel Solà.

11. Electronic Structure: Principles and Applications (ESPA 2002).

Sevilla, Spain; September 11-13, 2002.

-***Poster:*** "*Topological analysis of the electronic rearrangements along the reaction path by means of the ELF and AIM techniques*", Jordi Poater, Miquel Solà, Xavier Fradera, Miquel Duran, and Victor Polo.

-***Poster:*** "*Analysis of the carbon-lithium pair bond in CH_3Li and $(CH_3Li)_4$ systems by using the ELF and AIM methods*", E. Matito, Jordi Poater, Xavier Fradera, Miquel Duran, and Miquel Solà.

-***Poster:*** "*A new indicator of aromaticity based on the atoms in molecules delocalization index. Application to bowl-shaped polycyclic aromatic hydrocarbons*", Miquel Solà, Jordi Poater, Miquel Duran, and Xavier Fradera.

12. Theoretical Biophysics Symposium.

San Sebastian, Spain; March 5-7, 2003.

-***Communication:*** "*A new vision of aromaticity through the electron-pair density*", Jordi Poater, Miquel Solà, Xavier Fradera, and Miquel Duran.

-***Poster:*** "*Bond characterization of a series of Fischer-type Chromium-Carbene complexes by means of electron pairing analysis*", Jordi Poater, Montserrat Cases, Xavier Fradera, Miquel Duran, and Miquel Solà.

13. XIX meeting of the theoretical chemistry net of Catalonia.

Girona, Spain; July 17-18, 2003.

-***Communication:*** "*Bielectronic study of the hydrogen bond in the framework of the Atoms in Molecules theory*", Jordi Poater, Xavier Fradera, Miquel Solà, Miquel Duran, and Sílvia Simon.

14. VI Girona Seminar on Molecular Similarity.

Girona, Spain; July 21-24, 2003.

-***Communication:*** "*Study of the overall electronic delocalization in buckminsterfullerene by means of electron pairing analysis*", Jordi Poater, Miquel Duran, and Miquel Solà.

15. XX meeting of the theoretical chemistry net of Catalonia.

Barcelona, Spain; July 12-13, 2004.

-***Poster:*** "*Study of the local aromaticity of six-membered rings in pyracylene*", Jordi Poater, Miquel Solà, Rosario G. Viglione, and Ricardo Zanasi.

16. Electronic Structure Principles and Applications (ESPA 2004).

Valladolid, Spain; September 15-17, 2004.

-***Conference:*** "*Aromaticity quantified from the Atoms in Molecules delocalization indices*", Miquel Solà, Eduard Matito, Miquel Duran, Xavier Fradera, and Jordi Poater.

-***Poster:*** "*Is the NICS index a good indicator or aromaticity in pyracylene?*", Jordi Poater, Rosario G. Viglione, Ricardo Zanasi, and Miquel Solà.

17. Pomeranian quantum chemistry workshop. Electronic structure of atoms and molecules.

Pobierowo, Poland; May 12-15, 2005.

-***Communication:*** "*Electron correlation on chemical bonding descriptors*", Eduard Matito, Jordi Poater, Bernard Silvi, Lluis Blancafort, Miquel Duran, and Miquel Solà.

18. 11th international conference on the applications of density functional theory in chemistry and physics.

Geneve, Switzerland; September 11-15, 2005.

-***Poster:*** "*An aromaticity analysis of lithium-cation/π complexes of aromatic systems*", Mireia Güell, Jordi Poater, Josep M. Luis, Otilia Mo, Manuel Yañez, and Miquel Solà.

19. Evert Jan Baerends Symposium.

Amsterdam, The Netherlands; November 4, 2005.

-***Conference:*** "*Local aromaticity quantified using electron delocalization measures. Comparison with other criteria of aromaticity*", Miquel Solà, Miquel Duran, Eduard Matito, and Jordi Poater.

20. NWO/CW congress of theory and spectroscopy.

Lunteren, The Netherlands; January 30-31, 2006.

-***Poster:*** "*Hydrogen-hydrogen bonding in planar biphenyl, predicted by atoms-in-molecules, does not exist*", Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt.

-***Poster:*** "*Solvent effects on DNA base pairing*", Jordi Poater, Marcel Swart, Celia Fonseca-Guerra, and F. Matthias Bickelhaupt.

21. Chemical reactivity. A three day international conference on theoretical aspects of reactivity.

Brussels, Belgium; April 5-7, 2006.

-***Conference:*** "*Electron delocalization in aromatic molecules*", Miquel Solà , Ferran Feixas, Eduard Matito, and Jordi Poater.

-***Poster:*** "*Atoms-in-molecules theory wrongly predicts hydrogen-hydrogen bonding in planar biphenyl*", Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt.

22. VII Girona seminar on the nature of the chemical bond.

Girona, Spain; July 10-13, 2006.

-***Communication:*** "*Phenanthrene is more stable than anthracene due to more efficient pi-bonding, not H-H bonding*", Jordi Poater, Ruud Visser, Miquel Solà, and F. Matthias Bickelhaupt.

23. Electronic structure: Principles and applications.

Santiago de Compostela, Spain; July 18-21, 2006.

-***Poster:*** "*Atoms-in-molecules fails at assigning hydrogen-hydrogen bonding in planar biphenyl*", Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt.

24. 232nd ACS National Meeting.

San Francisco, USA; September 9-15, 2006.

-***Conference:*** "*New electron delocalization-based aromaticity criteria*", Jordi Poater, Eduard Matito, Ferran Feixas, Miquel Duran, and Miquel Solà.

-***Conference:*** "*Nonexistance of hydrogen-hydrogen bonding in planar biphenyl and the failure of Atoms-in-Molecules theory*", Jordi Poater, Miquel Solà, and F. Matthias Bickelhaupt.

25. XLI Congreso Mexicano de Química.

Mexico D. F., Mexico; September 24-28, 2006.

-***Conference:*** "Does H···H bonding in polycyclic aromatic hydrocarbons as predicted by the AIM theory exist? The case of biphenylene and phenanthrene", Miquel Solà, Jordi Poater, and F. Matthias Bickelhaupt.

26. Donostia physical chemistry symposium.

Donosti, Spain; December 11, 2006.

-***Conference:*** "Indicators of aromaticity based on the study of electron delocalization", Miquel Solà, Ferran Feixas, Eduard Matito, and Jordi Poater.

27. Energetics in chemistry. Central European school on physical organic chemistry.

Karpacz, Poland; June 4, 2007.

-***Conference:*** "Electronic aromaticity indexes", Eduard Matito, Ferran Feixas, Jerzy Cioslowski, Jordi Poater, and Miquel Solà.

28. 234th ACS National Meeting.

Boston, USA; August 19, 2007.

-***Conference:*** "Analysis of the local aromaticity in natural nucleobases and their size-expanded benzo-fused derivatives", Jordi Poater, Oscar Huertas, Miguel Fuentes-Cabrera, Modesto Orozco, Miquel Solà, and F. Javier Luque.

-***Conference:*** "DNA replication: Estimating the effects and interplay of solvation, pi-stacking and hydrogen bonding", Jordi Poater, Marcel Swart, Celia Fonseca-Guerra, and F. Matthias Bickelhaupt.

-***Conference:*** "Attractive or repulsive character of the halogen-halogen interaction in halogen-substituted biphenyls?", Jordi Poater, Joseph J. Dannenberg, F. Matthias Bickelhaupt, and Miquel Solà.

29. DFT2007: 12th International conference on the applications of density functional theory.

Amsterdam, The Netherlands; August 26, 2007.

-***Poster:*** "Estimating the effects and interplay of solvation, pi-stacking and hydrogen bonding in DNA replication", Jordi Poater, Marcel Swart, Celia Fonseca-Guerra, and F. Matthias Bickelhaupt.

-***Poster:*** "Electronic aromaticity measures from DFT calculations", Eduard Matito, Ferran Feixas, Jerzy Cioslowski, Jordi Poater, and Miquel Solà.

30. 37th Inorganic reaction mechanism group meeting.

Barcelona, Spain; January 9, 2008.

-***Conference:*** "Is the aromaticity of the benzene ring in the $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ complex larger than that of the isolated benzene molecule?", Miquel Solà, Ferran Feixas, J. Oscar C. Jiménez-Halla, Eduard Matito, and Jordi Poater.

31. 2008 Molecular informatics and bioinformatics.

Budapest, Hungary; March 26, 2008.

-***Conference:*** "The aromaticity puzzle: How can one assess the quality of the information extracted from different indicators of aromaticity?", Miquel Solà, Ferran Feixas, Eduard Matito, and Jordi Poater.

32. 236th ACS National Meeting.

Philadelphia, USA; August 17, 2008.

-***Conference:*** "A critical assessment on the performance of some aromaticity indices", Jordi Poater, Ferran Feixas, Eduard Matito, and Miquel Solà.

-***Conference:*** "Effects of solvation, pi-stacking, and hydrogen bonding on selectivity in DNA replication mechanism", Jordi Poater, Marcel Swart, Celia Fonseca-Guerra, and F. Matthias Bickelhaupt.

33. 6th Congress on electronic structure: principles and applications – ESPA 2008.

Palma de Mallorca, Spain; September 2, 2008.

-***Poster:*** "DNA replication mechanism: effects of solvation, pi-stacking, and hydrogen bonding on the selectivity", Jordi Poater, Marcel Swart, Celia Fonseca-Guerra, and F. Matthias Bickelhaupt.

34. 13th International congress of quantum chemistry, ICQC.

Helsinki, Finland; June 22, 2009.

-***Poster:*** "A critical assessment on the performance of some aromaticity indices", Ferran Feixas, Eduard Matito, J. Oscar C. Jiménez-Halla, Jordi Poater and Miquel Solà.

35. 13th International symposium on novel aromatic compounds, ISNA13.

Luxembourg, Luxembourg; July 19, 2009.

-***Poster:*** "A critical assessment on the performance of some aromaticity indices", Jordi Poater, Ferran Feixas, Eduard Matito, and Miquel Solà.

36. 240th ACS National Meeting.

Boston, USA; August 22, 2010.

-***Conference:*** "Patterns of π-electron delocalization in aromatic and antiaromatic organic compounds in the light of the Hückel's 4n+2 rule", Jordi Poater, Ferran Feixas, Eduard Matito, and Miquel Solà.

-***Conference:*** "A test to evaluate the performance of aromaticity descriptors in all-metal and semimetal clusters. An appraisal of electronic and magnetic indicators of aromaticity", Jordi Poater, Ferran Feixas, J. Óscar. Jiménez-Halla, Eduard Matito, and Miquel Solà.

37. CHITEL 2010.

Anglet, France; September 19, 2010.

-***Conference:*** "Performance of some widely used aromaticity indices. Can pi-electron delocalization patterns help us to define better indices?", Miquel Solà, Ferran Feixas, Eduard Matito, and Jordi Poater.

38. 241st ACS National Meeting.

Anaheim, USA; March 26, 2011.

-***Conference:*** "Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character", Jordi Poater, Ferran Feixas, Eduard Matito, Miquel Duran and Miquel Solà.

39. ***Ninth Triennal Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011).***
    Santiago de Compostela, Spain; July 17, 2011.
    -***Conference (invited):*** "Analysis of the selectivity in the DNA replication mechanism through solvation, pi-stacking and hydrogen bonding effects", Jordi Poater, Marcel Swart, Célia Fonseca-Guerra, and F. Matthias Bickelhaupt.
    -***Conference (invited):*** "Recent advances in the aromaticity of inorganic clusters and fullerenes", Miquel Solà, Ferran Feixas, Eduard Matito, and Jordi Poater.
    -***Poster:*** "On the relative stability of the XAAX and X_2A_2 isomers (X = H, F, Cl, Br, I, Li, Na; A = S, O)", Majid El Hamdi, Jordi Poater, F. Matthias Bickelhaupt, and Miquel Solà.
40. ***Excited states and non-adiabatic processes in complex systems. Theoretical approaches.***
    Sant Feliu de Guíxols, Spain; July 25, 2011.
    -***Poster:*** "Relative stability of XAAX and its isomer X_2A_2 (X = H, F, Cl, Br, I, Li, Na; A = S, O) through density functional theory", Majid El-Hamdi, Jordi Poater, F. Matthias Bickelhaupt, and Miquel Solà.
41. ***70th Birthday symposium of professor Joe Dannenberg.***
    New York, USA; September 16, 2011.
    -***Poster:*** "Aromaticity and electronic delocalization in all-metal clusters with single, double and triple aromatic character", Miquel Solà, Ferran Feixas, Eduard Matito, and Jordi Poater.
    -***Poster:*** "Stability of XAAX and X_2A_2 isomers (X = H, F, Cl, Br, I, Li, Na; A = S, O) through Kohn-Sham MO theory and energy decomposition analysis", Jordi Poater, Majid El-Hamdi, F. Matthias Bickelhaupt, and Miquel Solà.
42. ***I Meeting of the RSEQ Chemical Biology Group.***
    Santiago de Compostela, Spain; March 8, 2012.
    -***Communication and Poster:*** "Role of hydrogen bonding, pi-stacking and solvation on stacked DNA base pairs", Jordi Poater, Marcel Swart, Célia Fonseca Guerra and F. Matthias Bickelhaupt.
43. ***XXVIII Annual Meeting of the Theoretical and Computational Network of Catalonia.***
    Barcelona, Spain; June 11, 2012.
    -***Conference (invited):*** "From all-metal aromatic clusters to open-shell spherical aromaticity", Jordi Poater, Ferran Feixas, Eduard Matito and Miquel Solà.
44. ***VIIIth Congress on Electronic Structure: Principles and Applications (ESPA 2012).***
    Barcelona, Spain; June 26, 2012.
    -***Poster:*** "Solvation effects on DNA mismatches. How chlorouracyl mimics thymine in Escherichia Coli", Jordi Poater, Marcel Swart, Célia Fonseca Guerra and F. Matthias Bickelhaupt.
45. ***IDIBELL Cancer Conference on Personalized Cancer Medicine.***
    Bellvitge-Barcelona, Spain; December 3, 2012.
    -***Poster:*** "Selectivity in DNA replication. Quantum chemical study of primer extension", Jordi Poater, Marcel Swart, Célia Fonseca Guerra and F. Matthias Bickelhaupt.
46. ***International Conference on Chemical Bonding.***
    Kauai, USA; July 4, 2013.
    -***Conference:*** "Aromaticity in fullerenes and endohedral metallofullerenes. Effects on electronic structure, molecular structure and reactivity", Miquel Solà, Marc Garcia-Borràs, Sílvia Osuna, Jordi Poater, Marcel Swart, Josep M. Luis.
47. ***XXXIV Biannual Meeting of the Royal Spanish Society of Chemistry.***
    Santander, Spain; September 15, 2013.
    -***Conference:*** "The role of pi-pi interactions, H-bonding, twist angle and solvation in the stability of B-DNA structure", Jordi Poater, Marcel Swart, Célia Fonseca Guerra and F. Matthias Bickelhaupt.
    -***Conference:*** "Aromaticity in fullerenes and endohedral metallofullerenes. Effects on electronic structure, molecular structure and reactivity", Miquel Solà, Marc Garcia-Borràs, Sílvia Osuna, Jordi Poater, Marcel Swart, Josep M. Luis.
48. ***XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications.***
    Girona, Spain; June 30, 2014.

-***Conference (invited):*** "B-DNA structure and stability: The role of hydrogen bonding, pi-pi stacking interactions, twist angle and solvation", Jordi Poater, Marcel Swart, F. Matthias Bickelhaupt and Célia Fonseca Guerra.

49. Dutch Astrochemistry Network meeting.

Amsterdam, The Netherlands; December 4, 2014.

-***Conference (invited):*** "How do (exo)planetary environments affect chemistry?", Jordi Poater, Célia Fonseca Guerra, and F. Matthias Bickelhaupt.

50. 16th International Symposium on Novel Aromatic Compounds (ISNA2015).

Madrid, Spain; July 5, 2015.

-***Poster:*** "B-DNA structure and stability: The role of hydrogen bonding, pi-pi stacking interactions, twist-angle, and solvation", Jordi Poater, Célia Fonseca Guerra, and F. Matthias Bickelhaupt.

51. International Caparica Christmas Congress on Translational Chemistry.

Caparica, Portugal; December 7, 2015.

-***Conference (invited):*** "The role of hydrogen bonding, pi-pi stacking interactions, twist-angle, and solvation in B-DNA structure and stability", Jordi Poater, Célia Fonseca Guerra, and F. Matthias Bickelhaupt.

52. Festival of Genomics.

London, Great Britain; January 30, 2016.

-***Poster:*** "Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins", Jordi Poater, F. Matthias Bickelhaupt, and Jasmin Mecinovic.

53. 251st ACS National Meeting.

San Diego, USA; March 13, 2016.

-***Conference:*** "Aromaticity criteria based on electron delocalization measures", Jordi Poater.

-***Conference:*** "Role of hydrogen bonding, pi-pi stacking interactions, twist angle, and solvation on B-DNA", Jordi Poater.

-***Conference:*** "Close connection between pi aromaticity of hydrocarbons and three-dimensional aromaticity of closo boron hydrides", Jordi Poater.

54. Girona Seminar. Predictive Catalysis: Transition-metal reactivity by design.

Girona, Spain; April 17, 2016.

-***Poster:*** "Electronic structure and reactivity of donor-stabilized bis(amidinato/guanidinato) silylenes", Jordi Poater, Célia Fonseca Guerra, F. Matthias Bickelhaupt, and Reinhold Tacke.

55. 6th Euchems Chemistry Conference.

Sevilla, Spain; September 11, 2016.

-***Conference:*** "Aromaticity: a complex concept which may be made understood to the public", Jordi Poater.

56. XXXVI Reunión Bienal de la Real Sociedad Española de Química.

Sitges, Spain; June 25, 2017.

-***Communication:*** "B-DNA replication in non-terran biosolvents", Jordi Poater, Trevor A. Hamlin, Célia Fonseca Guerra, and F. Matthias Bickelhaupt.

-***Communication:*** "Everyday analogies to understand difficult concepts: Aromaticity", Sílvia Simon, Jordi Poater, Miquel Duran, and Miquel Solà.

-***Communication:*** "The Baird rule and the aromaticity of low-lying excited states", Miquel Solà, Ouissam El-Bakouri, Jordi Poater, and Ferran Feixas.

57. Modeling Interaction in Biomolecules VIII.

Pilsen, Czech Republic; September 3, 2017.

-***Conference (invited):*** "How non-terran bio-solvents affect the structure and stability of B-DNA", Jordi Poater, Trevor A. Hamlin, Célia Fonseca Guerra, and F. Matthias Bickelhaupt.

58. EMN Meeting on computation and theory 2017.

Dubai, United Arab Emirates; November 6, 2017.

-***Conference (invited):*** "Bridge between the aromaticity of polycyclic aromatic hydrocarbons and closo borohydrides", Jordi Poater, Miquel Solà, Clara Viñas, Francesc Teixidor.

59. Second International Christmas Caparica Congress in Translational Chemistry (IC3TC-2017).

Lisbon, Portugal; December 4, 2017.

-***Conference (invited):*** "Aromaticity of closo boron hydride clusters is driven by Hückel's rule", Jordi Poater, Miquel Solà, Clara Viñas, Francesc Teixidor.

60. H2020 Materials Networking School.

Sofia, Bulgaria; March 21, 2018.

-***Conference (invited):*** "Computer-aided analysis of the structure and stability of B-DNA: towards the design of supramolecular self-assembling materials", Jordi Poater.

61. Predictive Catalysis: Transition-Metal Reactivity by Design (Girona Seminar 2018).

Girona, Spain; April 3, 2018.

-***Poster:*** "Structure and stability of B-DNA model systems in non-terran bio-solvents", Jordi Poater, Trevor A. Hamlin, Célia Fonseca Guerra, and F. Matthias Bickelhaupt.

-***Communication:*** "Teaching Fe to behave like Pd in catalytic bond activation based on the activation strain model", Xiaobo Sun, Marcus V. J. Rocha, Jordi Poater, and F. Matthias Bickelhaupt.

-***Poster:*** "The Baird rule in all its guises", Miquel Solà, Ouissam El Bakouri, Jordi Poater, and Ferran Feixas.

62. I Latin American Conference on Chemical Bonding.

Sao Paulo, Brazil; June 10, 2018.

-***Conference (invited):*** "Design of supramolecular self-assembling materials derived from B-DNA nano-switches", Jordi Poater.

63. Second European Symposium on Chemical Bonding.

Oviedo, Spain; September 3, 2018.

-***Conference (invited):*** "Aromaticity of closo boron hydride clusters linked to polycyclic aromatic hydrocarbons via Hückel's rule", Jordi Poater.

64. 3rd Workshop on Magnetically Induced Currents in Molecules.

Kragujevac, Serbia; September 23, 2018.

-***Conference (invited):*** "Closo boron hydride clusters versus polycyclic aromatic hydrocarbons", Jordi Poater.

65. Aromaticity 2018.

Riviera Maya, Mexico; November 28, 2018.

-***Conference (invited):*** "Role of aromaticity and H···H interactions in the stability of polycyclic aromatic hydrocarbons", Jordi Poater.

66. XXXVII Meeting of the Spanish Royal Society of Chemistry.

San Sebastián, Spain; May 26, 2019.

-***Conference:*** "Games with the Periodic Table to increase public awareness of science", Jordi Poater, Sílvia Simon, Miquel Solà, Miquel Duran.

67. The 18th International Symposium on Novel Aromatic Compounds (ISNA-18).

Sapporo, Japan; July 21, 2019.

-***Conference:*** "Hückel's rule categorizes aromatic closo-boron hydride clusters", Jordi Poater.

68. The 23rd International conference on "Horizons in Hydrogen Bond Research" (HBOND2019).

Amsterdam, The Netherlands; September 23, 2019.

-***Conference (invited):*** "Non-terran biosolvents model structure, stability and replication of B-DNA", Jordi Poater.

69. 3rd International Caparica Christmas Conference on Translational Chemistry 2019.

Lisbon, Portugal; December 2, 2019.

-***Conference (invited):*** "Open-shell Jellium aromaticity in metal clusters", Jordi Poater.

70. ICMAB Seminar 2021.

Bellaterra, Spain; April 19, 2021.

-***Conference (invited):*** "Too persistent to give up: Aromaticity in boron clusters survives radical structural changes", Jordi Poater.

71. Foro "Teófilo Hernando" de Jóvenes Investigadores (IX conferencia), Real Academia Nacional de Mecidina de España.

Madrid, Spain; April 22, 2021.

-***Conference (invited):*** "Mecanismo de reconocimiento molecular de la trimetil lisina mediante proteínas lectoras epigenéticas", Jordi Poater.

72. 3rd Webinar on "Catalysis, Chemical Engineering & Technology".

Virtual, UK; June 24, 2021.

-***Conference (invited):*** "Teaching iron to perform like palladium in cross coupling reactions", Jordi Poater.

73. RSEQ Symposium 2021.

Virtual, Spain; September 27, 2021.

-***Communication:*** "The non-covalent nido-cage···π-ring interaction between boron clusters and aromatic rings", Jordi Poater.

74. International Conference on Carbon Chemistry and Materials.

Virtual, Italy; November 15, 2021.

-***Conference (invited):*** "Non-covalent nido-cage···π-ring interaction", Jordi Poater.

75. Catalysis Science & Technology 10th Anniversary Symposium.

Virtual, UK; November 16, 2021.

-***Conference (invited):*** "How does iron perform in cross-coupling reactions compared to palladium?", Jordi Poater.

76. I Simposio de Jóvenes Investigadores, Real Academia Nacional de Medicina.

Madrid, Spain; November 17, 2021.

-***Conference (invited):*** "Mecanismo de reconocimiento molecular de la trimetil- lisina a partir de sistemas aromáticos fluorados", Jordi Poater.

77. 13th European Conference on Computational and Theoretical Chemistry.

Virtual, Greece; November 18, 2021.

- ***Conference:*** "Non-covalent Interaction between Boron Clusters and Aromatic Rings and Its Applications", Jordi Poater.

78. Pacifichem 2021.

Virtual, USA; December 15, 2021.

- ***Conference:*** "Nido cage-pi interaction: A new non-covalent interaction", Jordi Poater.

- ***Conference:*** "Survival of the aromaticity in boron clusters despite radical structural changes", Jordi Poater.

79. ACS National Meeting Spring 2022.

Virtual, USA; March 20, 2022.

- ***Conference:*** "From Closo to Nido Carboranes: Aromaticity in Boron Clusters Survives Radical Structural Changes", Jordi Poater.

80. 9th European Conference on Boron Chemistry.

Bellaterra, Spain; July 3, 2022.

-***Conference (invited):*** "Aromaticity in Boron Clusters Survives Radical Structural Changes", Jordi Poater.

81. PSI-K Conference 2022.

Lausanne, Switzerland; August 22, 2022.

- ***Conference:*** "Clar π-Sextet Rule Determines Aromaticity and Extrusion of Benzenoids Linked to [o-COSAN]−", Jordi Poater.

82. EuChems 2022.

Libon, Portugal; August 28, 2022.

-***Conference:*** "Cage–···Cage– interaction: Boron cluster-based noncovalent bond and its applications in solid-state materials", Jordi Poater.

83. Magnetically Induced Molecular Currents (MAGIC) 2022.

Cambridge, UK; September 11, 2022.

-***Conference (invited):*** "Persistent strong diatropic ring currents in aromatic closo- and nido-carboranes", Jordi Poater.

84. 11th Singapore International Chemistry Conference (SICC-11).

Singapore, Singapore; December 11, 2022.

-***Conference (invited):*** "Aromaticity and Extrusion of Benzenoids linked to [o-COSAN]-: Clar has the Answer", Jordi Poater.

85. 1a Reunió de Química Teòrica i Computacional.
Barcelona, Spain; January 30, 2022.
-***Poster:*** "3D and 2D aromaticies: Like oil and water? The case of benzocarborane derivatives and 3D/3D fusion", Jordi Poater.

86. II Simposio de Jóvenes Investigadores, Real Academia Nacional de Medicina.
Madrid, Spain; May 17, 2023.
-***Conference (invited):*** "Lectura y eliminación del análogo de fosfonio de la trimetillisina por proteínas epigenéticas", Jordi Poater.

87. XXXIX Reunión Bienal de la Real Sociedad Española de Química.
Zaragoza, Spain; June 25, 2023.
-***Conference:*** "Aromaticity and Extrusion of Benzenoids Linked to [o-COSAN]−: Clar has the answer", Jordi Poater.

88. IUPAC – CHAINS 2023.
The Hague, The Netherlands; August 20, 2023.
-***Conference:*** "Construction of Hybrid Conjugation via Boron Cage Extension", Jordi Poater.

89. 19th European Symposium on Organic Reactivity (ESOR2023).
Amsterdam, The Netherlands; September 19, 2023.
-***Conference:*** "Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings", Jordi Poater.

90. ICMAB Seminar 2021.
Bellaterra, Spain; April 19, 2021.
-***Conference (invited):*** "Too persistent to give up: Aromaticity in boron clusters survives radical structural changes", Jordi Poater.

91. 5th Workshop on Magnetically Induced Molecular Currents (MAGIC) 2024.
Frauenwörth, Austria; September 9, 2024.
-***Conference (invited):*** "Facile Construction of New Hybrid Conjugation via Boron Cage Extension", Jordi Poater.

92. 4th European Symposium on Chemical Bonding (CBOND2024).
Amsterdam, The Netherlands; September 24, 2024.
-***Conference (invited):*** "On the existence of collective interactions reinforcing the metal-ligand bond in organometallic compounds", Jordi Poater.

Master and Theses supervised

- Supervision of **PhD thesis** "Molecular modeling of radical organic systems of interest in quantum computing", **Sergi Betkohshvili,** University of Barcelona, 2023 – 2026.
- Supervision of **PhD thesis** "Cooperativity in DNA guanine-quadruplexes and rosettes", **David Almacellas,** University of Barcelona, 2019 – 2023 (defense in April 2024).
- Supervision of **PhD thesis** "Brownmillerite Calcium Ferrite, a Promising Perovskite-Related Material in the Degradation of a Tight Dye under Ambient Conditions", **Zahra Noori,** University of Barcelona & Damghan University Iran, 2022 – 2024 (defense in February 2024).
- Supervision of Master thesis "Study of organic diradicals derived from indolo[3,2-b]carbazole and extension to the design of organic fi-tetraradicals: influence of geometry, conjugation, aromaticity and spin multiplicity", **Sergi Betkohshvili,** University of Barcelona, 2023 – 2026.
- Supervision of **PhD thesis** "Electronic structure, chemical bonding, and electronic delocalization of organic and inorganic systems with tridimensional or excited state aromaticity", **Ouissam El Bakouri El Farri**, University of Girona, 2014 – 2017 (November 22, 2017).
- Supervision of master thesis "Evaluating the difference between Mills-Nixon and reversed Mills-Nixon effect in tris-annelated benzene structures", Ilana van Doorm, Vrije Universiteit Amsterdam (2016).

- Supervision of master thesis "DFT study of regioselective Heck reactions employing supramolecular interactions", Pim R. Linnebank, Vrije Universiteit Amsterdam (2015).
- Supervision of master thesis "Mills-Nixon effect through energy decomposition analysis", Ilana M. van Doorn, Vrije Universiteit Amsterdam (2015).
- Supervision of master thesis "Computational study of the Diels-Alder reaction", Hans de Bruijn, Vrije Universiteit Amsterdam (2015).
- Supervision of master thesis "Normal to abnormal rearrangement and NHC activation in three-coordinate iron(II) carbene complexes", Jakub Med, Vrije Universiteit Amsterdam (2014).
- Supervision of **PhD thesis** "On the use of energy decomposition analyses to unravel the origin of the relative stabilities of isomers", **Majid El Hamdi Lahfid**, University of Girona, 2009 – 2013 (October 15th).
- Supervision of **PhD thesis** "Analysis of chemical bonding and aromaticity from electronic delocalization descriptors", **Ferran Feixas**, University of Girona, 2006 – 2011 (February 4th).
- Supervision of master thesis "Theoretical investigation of the relative stability of XAAX and its isomer X_2A_2 (X = H, F, Cl, Br, I, Li, Na, and A = S, O)", Majid El Hamdi Lahfid, University of Girona (2009).
- Supervision of master thesis "Analysis of the electronic delocalization in aromatic systems", Ferran Feixas, University of Girona (2007).

Other relevant points / achievements

Scientific

- **My H-Index is 45, and my 186 publications have received more than 7.780 citations according to ISI Web of Knowledge.**
- **20 of my publications have been cited more than 100 times.**
- **I appear at Elsevier Author Database (Stanford Ranking), as top 2% cited researcher in 2022.**
- **I appear at Research.com as Best Scientists Chemistry Ranking at University of Barcelona**
- I appear as "Scientist" at the Essentials Science Indicators of the ISI Web of Knowledge (top 1% cited).
- Granted with more than 1.250.000 EUR obtained in research proposals.
- Referee of J. Org. Chem., J. Phys. Chem., J. Chem. Phys., Chem. Phys. Lett., Org. Lett., Theor. Chem. Acc., Organometallics, J. Am. Chem. Soc., Phys. Chem. Chem. Phys, and **Nature Comm.**
- Member of the American Chemical Society, 2006.
- Member of the Royal Spanish Chemical Society, 2008.
- Member of the Catalan Chemical Society, 2003.
- My paper **Chem. Rev. 2005, 105, 3911-3947** (cited > 600 times) was considered a **"Fast Moving Front"** paper in Chemistry in July and November 2007 by the ESI Science Indicators, and a **"Hot Paper"** by the American Chemical Society due to its high number of citations.
- Member of a consolidated research group by the Generalitat de Catalunya.
- My **Chem. Comm. 2011, *47*, 11647-11649** was considered **"Hot Article"** by the Royal Society of Chemistry and has appeared on both its blog and Twitter due to its relevance.
- My **Comp. Theor. Chem. 2012, 998, 57-63** was chosen for the Virtual Special Issue in celebration of the publication of issue 1000 of the journal.
- My **Soft Matter 2011, 7, 9922-9932** has been chosen for the front cover of the issue.
- My **Chem. Eur. J. 2013, 19, 4169-4175** has been considered "Very Important Paper" and has been the back cover of the issue.
- **Recent 2 front covers in JACS**: Journal of the American Chemical Society 2023, 145, 22527-22538. DOI: 10.1021/jacs.3c07335; Journal of the American Chemical Society 2020, 142, 9396-9407. DOI: 10.1021/jacs.0c02228.
- **Recent front covers in Chem. Comm., ChemPhysChem, Chem. Eur. J., Phys. Chem. Chem. Phys.:** ChemPhysChem 2020, 21, 1092-1100. DOI: 10.1002/cphc.202000132.; Chemistry A European Journal 2021, 27, 15616-15622. DOI: 10.1002/chem.202103544; Physical Chemistry Chemical Physics 2019, 21, 9651-9664, DOI: 10.1039/c8cp07671e.; Chemical Communications

2019, 55, 5559-5562, DOI: 10.1039/c9cc02067e.; Chemistry A European Journal 2016, 22, 7437-7443.

- Supervisor of the collaborative project on the brain stroke with the Neurology Department of Hospital Josep Trueta in Girona.
- Experience in the use of Supercomputers because of a project of 670.000 hours in Marenostrum (Barcelona) as a researcher in head; and 125.000 hours in SARA (Amsterdam).
- Research project submitted under the ERC Consolidator Grant and evaluated between the top 22-31% ones (2013).
- Review Editor of Frontiers in Theoretical and Computational Chemistry (2013).

Training

- Attendance to the European summerschool in quantum chemistry (ESQC-00), Riolo Terme, Italy, September 2000.
- Attendance to the I Seram Conference on Clinical Molecular Imaging, Madrid, Spain, February 2009.
- Attendance to the CECAM 3rd CP2K Tutorial, Zurich, Switzerland, June 2013.

Organization of scientific activities

- Vicesecretary of the Local Organizing Committee of the IX Girona Seminar: Electron density, density matrices, and density functional theory (July 2010).
- Secretary of the Local Organizing Committee of the X Girona Seminar on Theoretical and computational chemistry for the modeling of biochemical systems: From theory to applications (July 2012).
- Secretary of the Local Organizing Committee of the XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From theory to applications (June 2014).
- Co-Chair of the Annual meeting of the Reference Network of Theoretical and Computational Chemistry of Catalonia – XRQTC (July 2018).
- Organizer of the monthly Research Seminars at the Institute of Theoretical and Computational Chemistry of the University of Barcelona (
- Scientific Advisory Board of the ***9th European Conference on Boron Chemistry,*** Bellaterra, Spain; July 3, 2022.
- Scientific Advisory Board of the ***5th Workshop on Magnetically Induced Molecular Currents (MAGIC) 2024,*** Frauenwörth, Austria; September 9, 2024.

Lecturer

- Teaching experience in Bachelor of Science Degree in Chemistry, University of Girona, Assistant Professor, 160 hours, Jan-Sep 2004; Ramon y Cajal Researcher, 60 hours, 2008-2009; 60 hours, 2009-2010; 30 hours, 2010-2011 in Master in Theoretical Chemistry and Computation; 60 hours, 2011-2012 in Master in Theoretical Chemistry and Computation.
- Molecular Computational Chemistry, Master in Chemistry, Vrije Universiteit Amsterdam (2013-14), 10 ECTS.
- Molecular Computational Chemistry, Master in Chemistry, Vrije Universiteit Amsterdam (2014-15), 10 ECTS.
- Molecular Computational Chemistry, Master in Chemistry, Vrije Universiteit Amsterdam (2015-16), 10 ECTS.
- HRSMC Course: Molecular Modeling, Master & PhD students, Vrije Univesiteit Amsterdam (June 6-17, 2016), 4 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2016-17), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2016-17), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2017-18), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2017-18), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2018-19), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2018-19), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2019-20), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2019-20), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2020-21), 3 ECTS.

- End-of-degree Research Project, University of Barcelona (2020-21), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2021-22), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2021-22), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2022-23), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2022-23), 1 ECTS.
- Computational Resources, Degree in Chemistry, University of Barcelona (2023-24), 3 ECTS.
- End-of-degree Research Project, University of Barcelona (2023-24), 1 ECTS.
- Coordinator of the new Master in Computational Chemistry and Catalysis of the University of Girona (2012-13).
- Supervisor of research projects by students of the last year of the High School.

Awards and Prices

- Appointed member of the young forum of the Spanish Royal National Academy of Medicine (2021).
- EMBO short term fellowship (Sep. 2013 – Dec. 2013).
- AIRE-CTP2012 travel grant from the European Commission and the Generalitat de Catalunya (Feb. 2013 – May 2013).
- HPC Europa grant on SARA Supercomputer (Oct. 2012 – Nov. 2012).
- European Reintegration Grant from the European Commission, R+D project (Mar. 2009 – Feb. 2012).
- Research grant on Marenostrum Supercomputer (Marc. 2009 – Feb. 2010).
- Prestigious Ramón y Cajal tenure-track position 5-year contract from the Spanish Ministry of Science and Innovation (Jan. 2008 – Dec. 2012).
- Postdoctoral IntraEuropean Marie Curie Fellowship 2-year contract from the European Commission (Jan. 2006 – Dec. 2007).
- Postdoctoral fellowship from the Catalan Ministry of Education and Universities (Oct. 2004 – Dec. 2005).
- PhD in Chemistry with highest honours.
- PhD fellowship from the Catalan Ministry of Education and Universities (Jan. 2000 – Dec. 2003).
- BsC in Chemistry with first-class honours.

Other

- Language skills:
    - Spanish – Mother tongue
    - Catalan – Mother tongue
    - English – Good
    - French – Average
- Wide knowledge of techniques derived from web 2.0 and applied to the communication of science (LinkedIn, Facebook, Twitter, blogs, web pages,…). In charge of the web site and blog of the Institute of Computational Chemistry of the UdG (2008-2012)
- Member of the Scientific Culture and Digital Communication Cathedra of the University of Girona. Part of the team in charge of the organization of the Researcher's Night (European Commission), with experience on digital techniques applied to the communication of science.