

CURRICULUM VITAE ABREVIADO (CVA)

Part A. PERSONAL INFORMATION

First name	Jordi		
Family name	Poater		
Gender (*)	Male	Birth date (dd/mm/yyyy)	21/04/1977
ID number	40333180N		
e-mail	jordi.poater@ub.edu	URL Web	https://www.icrea.cat/Web/ScientificStaff/jordi-poater-teixidor-219355
Open Researcher and Contributor ID (ORCID) (*)	0000-0002-0814-5074		

(*) *Mandatory*

A.1. Current position

Position	ICREA Research Professor		
Initial date	01/12/2015		
Institution	Universidad de Barcelona		
Department/Center	Dpt. Química Inorgánica y Orgánica	Instituto de Química Teórica y Computacional (IQTUB)	
Country	Spain	Teleph. number	629756913
Key words	aromaticity, weak interactions, reactivity, molecular structure		

A.2. Previous positions

Period	Position/Institution/Country/Interruption cause
2014-2016	Senior Associate Researcher, Vrije Universiteit Amsterdam, The Netherlands
2013	Associate Researcher, Universitat de Girona, Spain
2008-2012	Ramón y Cajal Researcher, Universitat de Girona, Spain
2006-2007	Marie Curie Postdoc, Vrije Universiteit Amsterdam, The Netherlands
2004-2005	Postdoc, Vrije Universiteit Amsterdam, The Netherlands

A.3. Education

PhD, Licensed, Graduate	University/Country	Year
PhD in Chemistry	Universitat de Girona	2003
BsC in Chemistry	Universitat de Girona	1999

Part B. CV SUMMARY (*max. 5000 characters, including spaces*)

Scientific contributions

My research takes off from two main lines, which are interconnected and reinforce each other. First, the study of aromaticity in organic and metal systems, with tools derived from the electron-pair density, with the purpose of analyzing the electronic structure and molecular bonding in a wide range of molecular systems. The main focus now is the 3D aromaticity of boron clusters. I have also become an expert in the application of Kohn-Sham molecular orbital theory complemented with quantitative bond energy decomposition analyses to the analysis of non-covalent interactions in a wide set of systems. In particular, the study of the hydrogen bonding and cooperativity in DNA derived systems and relevant interactions and mechanism in epigenetics have centered my most recent research.

I have published 33 articles in the last 3 years, as the result of the last MINECO project granted. Most of them are in top journals in chemistry: *Angew. Chem. Int. Ed.* (4), *J. Am. Chem. Soc.*, *J. Org. Chem.* (3), *Comm. Chem.* (2), *JACS Au*, *Nature Comm.*, *Org. Lett.*, *Chem. Eur. J.* (7) or *Phys. Chem. Chem. Phys.* (2). All of them have been published in open access, with the commitment to make them available to the whole community. And overall, I have 173



publications (Web of Knowledge), which have received almost 7.000 citations (9% self-citations, and H-Index = 42), most of them in first quartile, and 18 publications with more than 100 citations. Moreover, I am listed as "Scientist" in the ISI Essential Science Indicators as proof of being among the most cited scientists.

I have delivered 10 invited lectures in international conferences along the last 5 years, and overall, I have participated in over 75 international scientific events, with 51 delivered lectures, 11 short communications and 35 posters. Also noteworthy is that throughout my scientific career I have been granted with over 700.000 euros in research funding. Importantly, in 2018 I was granted as *garante* in the María de Maeztu excellence call for the IQTCUB with 2 million €, which has just been renovated for the next 4 years.

My research involves international collaborations with: Jasmin Mecinović (Denmark, on cation- π interactions and biomolecular recognition in epigenetic systems), F. M. Bickelhaupt (The Netherlands, on chemical bonding analysis in catalytic systems), C. Lichtenberg (Germany, on reactivity of bismuth systems), H. Yan (China, on non-covalent interactions in carboranes), R. Chauvin (France, on azulenes); as well as local collaborations: M. Solà (Girona, on aromaticity of organic and metallic systems), F. Teixidor & C. Viñas (Barcelona, on stability and aromaticity of carboranes), J. M. Bofill (Barcelona, on aromaticity of biradical species).

Contributions to society

Along my whole career as researcher, I have been committed to transfer my scientific knowledge to society. In the different research centers I have been, I have been involved in the outreach activities: social networks, web pages, visit to schools, participation in EU Researcher's Night,... In particular, at IQTCUB, and under the María de Maeztu Grant, I have participated in the development of an app to easily visualize in 3D different chemical systems (ModMol) with the cell phone; delivered lectures in computational chemistry courses at basic and advanced levels to attract graduate students to undertake a master in our institute; participated in the organization of fairs with other research centers and companies to let graduate students know about our master and PhD studies and research. In addition, in 2021 I was appointed young member of the Real Academia Nacional de Medicina de España in a multidisciplinary forum to approach our research to society from different backgrounds.

Contributions to training of researchers

I have supervised 3 PhD thesis: Dr. Ferran Feixas (2011, now RyC in UDG), Dr. Majid El-Hamdi (2013, now in chemical industry in Morocco), Dr. Ouissam El-Bakouri (2017, now JdC in UDG); and I am now supervising 3 more: David Almacellas (beginning 2024, UB), Emna Rahali (2024, UB and University of Tunis el Manar), and Zahra Noori (2025, UB and Damghan University). In addition, in the last 5 years I have supervised one postdoc (2020-2021) and several graduate and master students. As a member of the Department of Inorganic and Organic Chemistry of the UB, I am committed to the supervision of the research project of two last-year graduate students per year.

Final reference is made to the teaching given at both undergraduate and Master degrees, both in Amsterdam (UVA) and in Barcelona (UB), that complements my proven ability to address research teams, with either undergraduate students, or Master, or Doctoral or Postdocs. And last, but not least, I am referee for American Chemical Society, Royal Society of Chemistry, Nature Chemistry, Wiley, American Institute of Physics, or Frontiers in Chemistry (associate editor too); and research grant reviewer for AGAUR, Agencia Estatal de Investigación, Agencia Chilena, National Science Centre Poland, or Xunta de Galicia.

Part C. RELEVANT MERITS (sorted by typology)

C.1. Publications

Total publications in Web of Science: 173 with 6973 citations, 18 publications with more than 100 citations. Publications in the last 5 years: 48.

Most recent and relevant publications for the proposal (10 of the last 3 years):

- **J. Poater**, C. Viñas, M. Solà, F. Teixidor, "3D and 2D aromatic units behave like oil and water in the case of benzocarborane derivatives", *Nat. Comm.* 2022, 13, 3844.



- J. Jian, D. Barkhatova, R. Hammink, P. Tinnemans, F.M. Bickelhaupt, **J. Poater***, J. Mecinović, "Through-space stabilization of imidazolium cation by aromatic rings", *J. Org. Chem.* 2022, 87, 7875-7883.
- J. Jian, R. Hammink, P. Tinnemans, F.M. Bickelhaupt, C.J. McKenzie, **J. Poater***, J. Mecinović, "Probing noncovalent interactions in [3,3]metaparacyclophanes", *J. Org. Chem.* 2022, 87, 6087-6096.
- J. Jian, R. Hammink, C.J. Mackenzie, F.M. Bickelhaupt, **J. Poater***, J. Mecinović, "Probing the Lewis acidity of boronic acids through interactions with arene substituents", *Chem. Eur. J.* 2022, 28, e202104044.
- **J. Poater**, C. Viñas, D. Olid, M. Solà, F. Teixidor, "Aromaticity and extrusion of benzenoids linked to [o-COSAN]. Clar has the answer", *Angew. Chem. Int. Ed.* 2022, 61, e202200672.
- D. Tu, J. Li, F. Sun, H. Yan, **J. Poater***, M. Solà, "Cage···cage⁻ interaction: Boron cluster based non-covalent bond and its applications in solid-state materials", *J. Am. Chem. Soc. Au* 2021, 1, 2047-2057.
- K. Oberdorf, A. Hanft, J. Ramler, I. Krummenacher, F.M. Bickelhaupt, **J. Poater***, C. Lichtenberg, "Bismuth amides mediate facile and highly selective Pn-Pn radical coupling reactions (Pn = N, P, As)", *Angew. Chem. Int. Ed.* 2021, 60, 6441-6445.
- **J. Poater**, C. Viñas, I. Bennour, S. Escayola, M. Solà, F. Teixidor, "Too persistent to give up: Aromaticity in boron clusters survives structural changes", *J. Am. Chem. Soc.* 2020, 142, 9396-9407.
- D. Tu, H. Yan, **J. Poater***, M. Solà, "nido-cage···pi-bond: A non-covalent interaction between boron clusters and aromatic rings and its applications", *Angew. Chem. Int. Ed.* 2020, 59, 9018-9025.
- N. Savoo, J. Z. A. Laloo, L. Rhyman, P. Ramasami, F. M. Bickelhaupt, **J. Poater***, "Activation strain analyses of counterion and solvent effects on the ion-pair S_N2 reaction of NH₂⁻ and CH₃Cl", *J. Comput. Chem.* 2020, 41, 317-327.

C.2. Congress, indicating the modality of their participation (invited conference, oral presentation, poster)

Most recent invited lectures (10 of the last 5 years):

- 11th Singapore International Chemistry Conference, Singapore, December 2022, invited: "Aromaticity and extrusion of benzenoids linked to [o-COSAN]: Clar has the answer".
- 4th Workshop on Magnetically Induced Currents in Molecules (MAGIC2022), Cambridge, UK, September 2022, invited: "Persistent strong diatropic ring currents in aromatic closo- and nido-carboranes".
- 9th European Conference on Boron Chemistry, Barcelona, Spain, July 2022, invited and member of Scientific Organizing Committee: "Aromaticity in boron clusters survives radical structural changes".
- International Conference on Carbon Chemistry and Materials, Virtual, November 2021, invited: "Non-covalent nido-cage···π-ring interaction".
- 3rd International Caparica Christmas Conference on Translational Chemistry, Lisbon, Portugal, December 2019, invited: "Open-shell Jellium aromaticity in metal clusters".
- The 23rd International Conference on "Horizons in Hydrogen Bond Research" HBOND2019, Amsterdam, The Netherlands, September 2019, invited: "Chemically Controlled DNA Nanoswitch: Alkali Cations Pull the Lever in Various Solvents".
- The 18th International Symposium on Novel Aromatic Compounds (ISNA-18), Sapporo, Japan, July 2019, oral: "Hückel's rule categorizes Aromatic Closo-Boron Hydride Clusters".
- Aromaticity 2018, Riviera Maya, Mexico, November 2018, invited: "Role of aromaticity and H···H interactions in the stability of polycyclic aromatic hydrocarbons".
- 3rd Workshop on Magnetically Induced Currents in Molecules, Kragujevac, Serbia, September 2018, invited: "Closo Boron Hydride Clusters versus Polycyclic Aromatic Hydrocarbons".
- Second European Symposium on Chemical Bonding, Oviedo, Spain, September 2018, invited: "Aromaticity of Closo Boron Hydride Clusters linked to Polycyclic Aromatic Hydrocarbons via Hückel's Rule".



C.3. Research projects, indicating your personal contribution. In the case of young researchers, indicate lines of research for which they have been responsible.

- María de Maeztu unit of excellence award for IQTCUB, Ministerio de Ciencia e Innovación (CEX2021-001202-M), Researcher, PI: Eliseo Ruiz, Universitat de Barcelona, Spain (2023-2026), 2.000.000 EUR.
- Grupo de investigación consolidado, Generalitat de Catalunya (2021SGR00442), **Co-PI: J. Poater**, Universitat de Barcelona & ICMA B, Spain (2023-2024), 40.000 EUR.
- “Modelado de interacciones no-covalentes y cooperatividad en pares de bases de ADN (no)naturales y en cudruplexes de guanina” (PID2019-106830GB-I00), Ministerio de Ciencia e Innovación (MINECO), **PI: J. Poater**, Universitat de Barcelona, Spain (2020-2023), 60.500 EUR.
- María de Maeztu unit of excellence award for IQTCUB, Ministerio de Ciencia, Innovación y Universidades (MDM-2017-0767), **Co-PI (garante): J. Poater**, Universitat de Barcelona, Spain (2018-2022), 2.000.000 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), 36.000 EUR.
- “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: J. Poater**, Vrije Universiteit Amsterdam, The Netherlands (2014-2017), 226.121 EUR.
- “Silicon alpha-effect: a systematic experimental and computational study of the hydrolysis of functionalizedalkoxytriorganylsilanes”, **PI: J. Poater**, Wacker Chemie AG, Vrije Universiteit Amsterdam, The Netherlands (2014-2015), 55.000 EUR.
- “*Reactivity and chemical bonding in biomedicine and (bio)inorganic chemistry*” (CTQ2008-06532/BQU, Spanish Education and Science Ministry), Researcher, PI: Dr. Marcel Swart, ICREA and Institute of Computational Chemistry, University of Girona (2009-2011).
- “*Quantum biochemistry: DNA replication and biomolecular recognition*” (Ramón y Cajal, Spanish Education and Science Ministry), **PI: J. Poater**, Institute of Computational Chemistry, University of Girona (2008-2012), 189.000 €.
- “*Quantumbiology: DNA replication and biomolecular recognition*” (European Reintegration Grant, European Commission), **PI: J. Poater**, Institute of Computational Chemistry, University of Girona (2009-2012), 45000 €.

C.4. Other merits

Organization of scientific events

- Member of the Scientific Organizing Committee, 9th European Conference on Boron Chemistry (EuroBoron), Barcelona, Spain (July 2022).
- Secretary of the organizing committee of the XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From theory to applications, Girona, Spain (June 2014, 100 participants).
- Secretary of the organizing committee of the X Girona Seminar on Theoretical and computational chemistry for the modeling of biochemical systems: From theory to applications, Girona, Spain (July 2012, 140 participants, including Nobel Prize A. Warshel).
- Secretary of the organizing committee of the IX Girona Seminar: Electron density, density matrices, and density functional theory, Girona, Spain (July 2010, 100 participants).

Distinctions

- *Garante* in María de Maeztu excellence grant for IQTCUB (2M EUR).