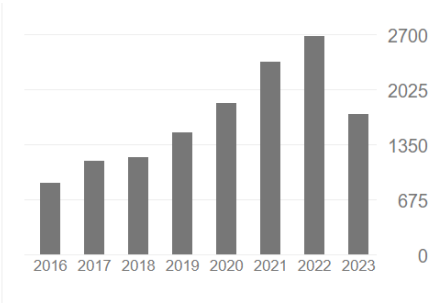
CV Julia Contreras-García

Affiliation: CNRS at Sorbonne Université
Current position at CNRS: Directrice de recherche
Current position at Sorbonne: Team leader of the Chemical Interpretation team at Laboratoire de Chimie Théorique

E-mail: contrera@lct.jussieu.fr
Gender : F
Nationality: Spanish

http://www.lct.jussieu.fr/pagesperso/contrera/index.html



CITATION RECORDS

(Google Scholar 11/07/2023)

Publications: 112

Total times cited: 15290

H-index: 36

Age : 43 years old

Summary

My research career could be summarized in the words “Chemical Bond”. I started working on chemical bond during my PhD, mainly on electron localization in strong bonds in the solid state. During my postdoc at Duke University, I moved towards non-covalent interactions and biosystems. I am now 42 years old and Directrice de Recherche (CNRS- Full Professor rank) leading the Chemical Interpretation group in Sorbonne Université. Here, I have merged all these fields and I focus on developing new approaches to understand complex properties from topological definitions of the chemical bond. This approach has shown to be very successful in understanding such complex properties as **catalysis, photochemistry, enantionselectivity and biomolecular interactions**.

In each case, this has required developing appropriate indexes and electronic structure-property relationship. Most noticeably, I am probably best identified for my work in NCI (Non-Covalent Interaction Index), which enables visualization of non-covalent interactions, which was also published in **J. Am. Chem. Soc (over 5600 citation**s). I also wrote the program to analyze this index, **NCIPLOT**. The associated paper was published in 2011 in JCTC and was among **the top 10 most read JCTC** papers this year. It has received over 2600 citations and more than 13000 visits. Most recently my interests have turned into electron localization in the solid state again and its relationship with superconductivity. In this topic, I have been able to finally develop an index that describes superconductivity from fast calculations (**Nature Communications** 12, 5381 (2021)).

I have published **112 articles** (**1 Natur Comm, 3 JACS, 1 PRL, 5 Chem Eur J, 1 Chem Sci**), as well as two JCTC papers which entered the **10-most-read of their year** of publication. This is probably what I would like to highlight here. The works I endeavor in are usually methodological, so most typically, they go to specialized journals. Nevertheless, their relevance can be outlined by the number of citations, which I have added to the list below.

My dedication to the topic has been recently recognized by Springer, who invited me with a colleague to write a book on the topic (Topological approaches to the chemical bond, Springer 2023) which has just seen the light. In the same direction, **I was finalist for the Dirac medal (2nd place) by the**

WATOC committee in 2021. My contributions to solid state were recognized in 2013, when I received the **European High Pressure Award.**

From the institutional and activity viewpoint, I am glad to participate in several scientific societies. I am part of the **editorial board of CTC.** I am the **President of the European Committee of High Pressure** since 2022 (approx. 200 members). I have also been involved in the **creation of scientific associations** (European Committee of Chemical Bonding). I have also been very involved in the organization and coordination of initiatives to **promote women in science**. I have created the online database "Women under High Pressure". This has led to several public conferences and interventions in Conferences and the development of a permanent set of rules to promote women participation in IUCr conferences.

Finally, I would also like to mention as recognition index my participation in conferences as invited speaker. Taking this year into account I will have given 10 plenary talks (including the ICQC-theoretical chemistry conference) and 50 invited/keynote talks (including several Gordon, Telluride, Watoc and ACS).

I would not want to finish this summary without mentioning my mentoring activity. I have had the chance to mentor 13 PhD/postdocs over these years. In all cases I have focused on transmitting a good and enjoyable way of doing science. Those students who have finished are all now working, a big majority of them in academia…and they always come to visit the group hopefully leading to a durable school of Chemical Bond studies.

Publication summary

- **1 Text Book** - "Topological approaches to the chemical bond" by J. Contreras-Garcia and A. M. Pendas (Springer, 2023)
- 12 Book Chapters
- 112 articles (**1 Natur Comm, 3 JACS, 1 PRL, 5 Chem Eur J, 1 Chem Sci**)

10 Main publications in the last 10 years (112 in total) – citations on 11/07/2023

1. F. Belli, T. Novoa, J. Contreras-Garcia, I. Errea, "Strong correlation between electronic bonding network and critical temperature in hydrogen-based superconductors", **Nature Communications** 12, 5381 (2021) **29 citations** DOI:10.1038/s41467-021-25687-0
2. R. A. Boto, F. Peccati, R. Laplaza, C. Quan, A. Carbone, J.-P. Piquemal, Y. Maday, J. Contreras-Garcia*, "NCIPLOT4: Fast, Robust, and Quantitative Analysis of Noncovalent Interactions", J. Chem. Theory Comput. 16, 7, 4150 (2020) **120 citations** DOI: 10.1021/acs.jctc.0c00063
3. J. Klein, H. Khartabil, J.-C. Boisson, J. Contreras-Garcia, J.-P. Piquemal, E. Henon "A New Way for Probing Bond Strength", J. Phys. Chem. A,124, 1850 (2020) **102 citations** DOI:10.1002/cphc.201701325
4. J. Calvo, C. Weston, J. Contreras-Garcia,* M. J. Fuchter "Tuning Azoheteroarene Photoswitch Performance through Heteroaryl Design", **J. Am. Chem. Soc.** 139, 1261 (2017) **231 citations** DOI: 10.1021/jacs.6b11626
5. C. Lefebvre, H. Khartabil, J.-C. Boisson, J. Contreras-Garcia, J.-P. Piquemal, E. Henon, "Independent Gradient Model: a new approach for probing strong and weak interactions in molecules from wave function calculations" Chem Phys Chem (2017). **231 citations** DOI:10.1002/cphc.201701325
6. R. A. Boto, J.P. Piquemal, J Contreras-Garcia* "Revealing strong interactions with the reduced density gradient: a benchmark for covalent, ionic and charge-shift bonds", Theor Chem Acc 136 (2017) **96 citations** DOI: 10.1007/s00214-017-2169-9

7. C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-Garcia, E. Henon, "Accurately extracting the signature of intermolecular interactions present in the NCI plot of the reduced density gradient versus electron density", Phys Chem Chem Phys 19, 17928 (2017) **889 citations** DOI: 10.1039/C7CP02110K
8. A. Armstrong, R. A. Boto, P. Dingwall, J. Contreras-Garcia, M. J. Harvey, N. Mason, H. S. Rzepa, "The Houk-List Transition states for organocatalytic mechanism revisited", **Chem. Science,** 5, 2057 (2014) **171 citations** DOI: 10.1039/C3SC53416B
9. J. R. Lane, J. Contreras-Garcia*, J.-P. Piquemal, B. J. Miller, and H. G. Kjaergaard "Are Bond Critical Points Really Critical for Hydrogen Bonding?" J. Chem. Theory Comp. 9, 3263 (2013) **[Most read in JCTC 2013] 414 citations** DOI: 10.1021/ct400420r
10. M. Virshup, J. Contreras-Garcia, P. Wipf, W. Yang, D. N. Beratan "Stochastic Voyages into Uncharted Chemical Space Produce a Representative Library of All Possible Drug-Like Compounds" **J. Am. Chem. Soc.** 135, 7296 (2013) **252 citations** DOI : 10.1021/ja401184g

Invited conferences

I have enjoyed invitations to the main conferences in chemistry (ACS) and theoretical chemistry (e.g. ICQC, Watoc) as well as other well reknonwn conference series (Telluride, Gordon) and the conferences in my topics (IUCr, Sagamore)

Selection of Plenaries/keynotes (8 in total)

- ICQC (Slovakia, 2023)
- ICNI (France, 2022)
- ESPA (Vigo, 2022)
- IUCr (Prague, 2021)
- European High Pressure Research Group Meeting (London, UK, 2013). EHPRG Award Lecture

Selection of invited talks at conferences/schools (50 in total)

- IUCr (Melbourne, 2023)
- **Telluride** Intermolecular Interactions: New Challenges for ab initio Theory (Telluride, 2023)
- WATOC (Vancouver, 2022)
- **Bienal de Quimica** (Spain, 2022)
- Pacifichem (Online, 2021)
- Density Functional Theory and its Applications (Alicante, Spain, 2019)
- Scientific Computing Across Scales - Quantum Systems in Cold-matter Physics and Chemistry" (Fields Institute of Toronto, 2019)
- Sagamore (Halifax, 2018)
- **ACS** (New Orleans, 2018)
- **Erice** School on Quantum Crystallography (Erice, 2018)
- **Telluride** "Intermolecular Interactions: New Challenges for ab initio Theory" (Cabrales, 2017)
- **WATOC** (Munich, 2017)
- IUCr (India, 2017)
- ESPA (Castello, Spain, 2016)
- **WATOC** (Santiago de Chile, Chile, 2014)
- **Gordon Research Conference** in High Pressure (Main, USA, 2014)
- **Gordon Research Conference** in Electron Distribution and chemical bonding (Switzerland, 2013)
- 20th International Conference on Horizons in Hydrogen Bond Research (Antwerp, Belgium, 2013)

Conference and training session organization

- Erice School (Italy, 2025)
- CECAM (Lyon, 2023)
- CTTC (Trujillo, 2016)
- CTTC (Vietnam, 2014)
- RCTF (Paris, 2014)

Journal referee

Nature Communications, Chemistry European Journal, ACS Catalysis, Chemical Science, etc

Editor responsabilities and book contributions

Editorial board at the Computational and Theoretical Chemistry
Book "Topological approaches to the chemical bond" written by J. Contreras-Garcia and A. M. Pendas (Springer, 2023)

Prizes

- European High Pressure Research Group Award (2013)

Participation in committees and other responsabilities

- HCERES Expert Pannel member (2022-2025) – national evaluation of laboratories
- HCERES pannel member (2021)
- IQCC Scientific Advisory Board (2023-)
- FWO Chemistry pannel President (2021)
- Chair of the European High Pressure Research Society (EHPRG) (2022-2025)
- Secretary of the European High Pressure Research Society (EHPRG) (2018-2022)

Current Funding

- ANR (France), Position: PI (09/2022-08/2026), 303 k€
- ECOS biletaral project France-Chili, Position PI (01/2022-03/2026), 20k€
- H2020-Synergy, Position: member (02/2019-02/2026), 9900l€
- Emergence, Position: PI (09/2023-08/2025), 60.8k€
- ANR, Position: local PI (01/2024-06/2027), 47.8k€
- ANR, Position: member (10/2023-10/2026), 294k€

Public awareness & Outreach

- Creation of the European Community of Chemical Bonding (ECCB)
- Creation of Women under High Pressure group
- Organizer of the Power Hour for Womer in Science at the Gordon Research Conference in High Pressure 2016
- Creation of stories for El Monstrutren, science for kids.