Rubén Laplaza

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Curriculum Vitae
February 2023

Academic Record

2020 – *ongoing* **Postdoctoral fellow**, LCMD, EPFL (Switzerland)
Supervisor:
Prof. C. Corminboeuf (clemence.corminboeuf@epfl.ch)

2017 – 2020 **International Ph.D. in Theoretical Chemistry**, Sorbonne Université (France) & Universidad de Zaragoza (Spain)
Thesis title: *Semiquantitative Bond Models from Quantum Chemical Topology*.
Supervisors:
Prof. J. Contreras-García (contrera@lct.jussieu.fr),
Prof. V. Polo (vipolo@unizar.es)

2016 – 2018 **Master in Theoretical Chemistry and Computational Modelling**, Universidad de Santiago de Compostela (Spain)
Master Thesis title: *Densities and Energies: a Perspective From Quantum Chemical Topology*.
Supervisors:
Prof. J. Contreras-García (contrera@lct.jussieu.fr),
Dr. S. Vázquez (saulo.vazquez@usc.es)

2012 – 2016 **Chemistry Degree**, Universidad de Zaragoza (Spain)

Publications

Journal Articles

1. Novoa, T.; **Laplaza**, **R.**; Peccati, F.; Fuster, F.; Contreras-García, J. *J. Chem. Inf. Model.* **2023**, *63*, 4483–4489.
2. Wodrich, M. D.; **Laplaza**, **R.**; Cramer, N.; Reiher, M.; Corminboeuf, C. *CHIMIA* **2023**, *77*, 139.
3. Gallarati, S.; Gerwen, P. V.; Schoepfer, A. A.; **Laplaza**, **R.**; Corminboeuf, C. *CHIMIA* **2023**, *77*, 39.
4. Wieduwilt, E. K.; Boto, R. A.; Macetti, G.; **Laplaza**, **R.**; Contreras-García, J.; Genoni, A. *J. Chem. Theory Comput.* **2023**, *19*, 1063–1079.
5. **Laplaza**, **R.**; Das, S.; Wodrich, M. D.; Corminboeuf, C. *Nat. Protoc.* **2022**, *17*, 2550–2569.
6. Vela, S.; **Laplaza**, **R.**; Cho, Y.; Corminboeuf, C. *npj Comput. Mater.* **2022**, *8*, 188.
7. Das, S.; **Laplaza**, **R.**; Blaskovits, J. T.; Corminboeuf, C. *Angew. Chem. Int. Ed.* **2022**, *134*.
8. Jurásková, V.; Célerse, F.; **Laplaza**, **R.**; Corminboeuf, C. *J. Chem. Phys.* **2022**, *156*, 154112.
9. **Laplaza**, **R.**; Gallarati, S.; Corminboeuf, C. *Chemistry–Methods* **2022**, *2*, e202100107.
10. Schwaller, P.; Vaucher, A. C.; **Laplaza**, **R.**; Bunne, C.; Krause, A.; Corminboeuf, C.; Laino, T. *WIREs Comput. Mol. Sci.* **2022**, *12*, DOI: 10.1002/wcms.1604.
11. **Laplaza**, **R.**; Contreras-Garcia, J.; Fuster, F.; Volatron, F.; Chaquin, P. *Comput. Theor. Chem.* **2022**, *1207*, 113505.
12. Gallarati, S.; **Laplaza**, **R.**; Corminboeuf, C. *Org. Chem. Front.* **2022**, *9*, 4041–4051.
13. Gallarati, S.; van Gerwen, P.; **Laplaza**, **R.**; Vela, S.; Fabrizio, A.; Corminboeuf, C. *Chem. Sci.* **2022**, *13*, 13782–13794.
14. Garner, M. H.; **Laplaza**, **R.**; Corminboeuf, C. *Phys. Chem. Chem. Phys.* **2022**, *24*, 26134–26143.
15. Landeros-Rivera, B.; Gallegos, M.; Munarriz, J.; **Laplaza**, **R.**; Contreras-Garcia, J. *Phys. Chem. Chem. Phys.* **2022**, *24*, 21538–21548.

16 **Laplaza**, **R.**; Sobez, J.-G.; Wodrich, M. D.; Reiher, M.; Corminboeuf, C. *Chem. Sci.* **2022**, *13*, 6858–6864.

17 Romero-Tamayo, S.; **Laplaza**, **R.**; Velazquez-Campoy, A.; Villanueva, R.; Medina, M.; Ferreira, P. *Oxid. Med. Cell. Longev.* **2021**, *2021*, 1–19.

18 Gallarati, S.; Fabregat, R.; **Laplaza**, **R.**; Bhattacharjee, S.; Wodrich, M. D.; Corminboeuf, C. *Chem. Sci.* **2021**, *12*, 6879–6889.

19 **Laplaza**, **R.**; Cárdenas, C.; Chaquin, P.; Contreras-García, J.; Ayers, P. W. *J. Comput. Chem.* **2020**, *42*, 334–343.

20 **Laplaza**, **R.**; Peccati, F.; A. Boto, R.; Quan, C.; Carbone, A.; Piquemal, J.-P.; Maday, Y.; Contreras-García, J. *WIREs Comput. Mol. Sci.* **2020**, *11*.

21 Boto, R. A.; Peccati, F.; **Laplaza**, **R.**; Quan, C.; Carbone, A.; Piquemal, J.-P.; Maday, Y.; Contreras-García, J. *J. Chem. Theory Comput.* **2020**, *16*, 4150–4158.

22 **Laplaza**, **R.**; Contreras-Garcia, J.; Fuster, F.; Volatron, F.; Chaquin, P. *Chem. Eur. J.* **2020**, *26*, 6839–6845.

23 **Laplaza**, **R.**; Boto, R. A.; Contreras-García, J.; Montero-Campillo, M. M. *Phys. Chem. Chem. Phys.* **2020**, *22*, 21251–21256.

24 **Laplaza**, **R.**; Polo, V.; Contreras-García, J. *J. Phys. Chem. A* **2019**, *124*, 176–184.

25 Villanueva, R.; Romero-Tamayo, S.; **Laplaza**, **R.**; Martínez-Olivan, J.; Velázquez-Campoy, A.; Sancho, J.; Ferreira, P.; Medina, M. *Antioxid. Redox Signal.* **2019**, *30*, 2013–2029.

26 Peccati, F.; **Laplaza**, **R.**; Contreras-García, J. *The Journal of Physical Chemistry C* **2019**, *123*, 4767–4772.

27 **Laplaza**, **R.**; Polo, V.; Contreras-García, J. *Phys. Chem. Chem. Phys.* **2019**, *21*, 20927–20938.

28 Munárriz, J.; **Laplaza**, **R.**; Martín Pendás, A.; Contreras-García, J. *Phys. Chem. Chem. Phys.* **2019**, *21*, 4215–4223.

29 Munárriz, J.; **Laplaza**, **R.**; Polo, V. *Mol. Phys.* **2018**, *117*, 1315–1324.

30 Quero, J.; Cabello, S.; Fuertes, T.; Mármol, I.; **Laplaza**, **R.**; Polo, V.; Gimeno, M. C.; Rodriguez-Yoldi, M. J.; Cerrada, E. *Inorg. Chem.* **2018**, *57*, 10832–10845.

31 Martínez-Júlvez, M.; Goñi, G.; Pérez-Amigot, D.; **Laplaza**, **R.**; Ionescu, I.; Petrocelli, S.; Tondo, M.; Sancho, J.; Orellano, E.; Medina, M. *Molecules* **2017**, *23*, 29.

Books and Chapters

1 **Laplaza**, **R.**; Munárriz, J.; Contreras-García, J. In *Conceptual Density Functional Theory: Towards a New Chemical Reactivity Theory*; Wiley: 2022, pp. 349–374.

2 **Laplaza**, **R.**; Peccati, F.; Arias-Olivares, D.; Contreras-García, J. In *Complementary Bonding Analysis*; De Gruyter: 2021, pp. 353–378.

Congress Presentations

- NaviCat: Computational Tools to Navigate Molecular Catalyst Landscape — Poster, *12th WATOC Conference*, Vancouver, 2022.
- Localization of Density Errors in Density Functional Theory — Poster, *Quantum Crystallography Online Meeting 2020 (QCrOM2020)*, Online, 2020.
- Density Error Localization in Density Functional Theory — Poster, *Theoretical Chemistry and Computational Modeling: 20 years promoting Excellence in Science (20TCCM)*, San Sebastián, Spain, 2019.
- Electron density based analysis of noncovalent interactions in large systems: the NCIweb server — Flash Communication, *XXXVII Biennial Meeting of the Spanish Royal Society of Chemistry*, San Sebastián, Spain, 2019.
- Assessing densities through quantum chemical topology — Single Figure Presentation, *Virtual Winter School on Computational Chemistry*, 2019.
- The inverted C-C bond revisited: the case of [1.1.1]Propellane — Poster, 2^{nd} *European Symposium on Chemical Bonding (ESCB2)*, Oviedo, Spain, 2018.
- Densities and Energies: a Perspective from Quantum Chemical Topology — Poster, 11^{th} *Congress on Electronic Structure: Principles and Applications (ESPA2018)*, Toledo, Spain, 2018.

Congress Presentations (continued)

- Exploring Non-Covalent Interactions through Molecular Orbitals — Poster, 16^{th} *International Congress of Quantum Chemistry (16-ICQC)*, Menton, France, 2018.
- Energy Models from Quantum Chemical Topology — Oral presentation, 4^{th} *Luchon Tutorial in Theoretical Chemistry*, Luchon-Superbagneres, France, 2018.

Other Merits

Scientific Mobility

February 2020	Visiting student *(3 days)* at Université de Lorraine, under the supervision of Dr. Alessandro Genoni (`alessandro.genoni@univ-lorraine.fr`)
September 2019	Visiting student *(1 month)* at Universidad de Chile, Grupo de Física Atómica y Molecular, under the supervision of Dr. Carlos Cárdenas (`cardena@uchile.cl`)
June 2019	Visiting student *(3 months)* at McMaster University, Ayers Group, under the supervision of Prof. P.W. Ayers (`ayers@mcmaster.ca`)

Awards and Achievements

- European Master in Theoretical Chemistry and Computational Modelling special prize.
- LabEx MiChem Sorbonne Université mobility grant.
- Inscription grant from the GEQC of the Spanish Royal Society of Chemistry (RSEQ).
- Poster prize, *Quantum Crystallography Online Meeting 2020 (QCrOM2020)*

Teaching Experience *(in French)*

2018 – 2019	UE 1C001 : Chimie 1 – Structure et réactivité *(Chemistry 1 – Structure and reactivity)*
	UE 2A005 : Programmation pour le calcul scientifique *(Programming for scientific calculation)*
	UE 3C001 : Mécanique quantique et spectroscopies *(Quantum mechanics and spectrocopy)*
2019 – 2020	LU2CI005 : Spectroscopies *(Spectrocopy)*
	LU3CI001 : Mécanique quantique et spectroscopies *(Quantum mechanics and spectrocopy)*

Experience as Reviewer

2018 – *ongoing*	Referee for *J. Chem. Theory Comput.*, *Phys. Chem. Chem. Phys.*, *Digital Discovery* and other digital and computational chemistry journals.