Rubén Laplaza

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Curriculum Vitae
October 2024

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:
Dr. S. Vázquez (saulo.vazquez@usc.es),
Prof. J. Contreras-García (contrera@lct.jussieu.fr)

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

Publications

Preprints

1. Schoepfer, A., Weinreich, J., **Laplaza**, **R.**, Waser, J., & Corminboeuf, C. (2024). *Cost-informed bayesian reaction optimization* [http://dx.doi.org/10.26434/chemrxiv-2024-44ft2]. https://doi.org/10.26434/chemrxiv-2024-44ft2

Journal Articles

1. **Laplaza**, **R.**, Wodrich, M. D., & Corminboeuf, C. (2024). Overcoming the pitfalls of computing reaction selectivity from ensembles of transition states. *J. Phys. Chem. Lett.*, *15*(29), 7363–7370. https://doi.org/10.1021/acs.jpclett.4c01657

2. van Gerwen, P., Briling, K. R., Bunne, C., Somnath, V. R., **Laplaza**, **R.**, Krause, A., & Corminboeuf, C. (2024). 3dreact: Geometric deep learning for chemical reactions. *J. Chem. Inf. Model.* https://doi.org/10.1021/acs.jcim.4c00104

3. Schoepfer, A. A., **Laplaza**, **R.**, Wodrich, M. D., Waser, J., & Corminboeuf, C. (2024). Reaction-agnostic featurization of bidentate ligands for bayesian ridge regression of enantioselectivity. *ACS Catal.*, 9302–9312. https://doi.org/10.1021/acscatal.4c02452

4. Worakul, T., **Laplaza**, **R.**, Das, S., Wodrich, M. D., & Corminboeuf, C. (2024). Microkinetic molecular volcano plots for enhanced catalyst selectivity and activity predictions. *ACS Catal.*, 9829–9839. https://doi.org/10.1021/acscatal.4c01175

5. Das, S., **Laplaza**, **R.**, Blaskovits, J. T., & Corminboeuf, C. (2024). Engineering frustrated lewis pair active sites in porous organic scaffolds for catalytic co2 hydrogenation. *J. Am. Chem. Soc.*, *146*(23), 15806–15814. https://doi.org/10.1021/jacs.4c01890

6. Cho, Y., **Laplaza**, **R.**, Vela, S., & Corminboeuf, C. (2024). Automated prediction of ground state spin for transition metal complexes. *Digital Discovery*, *3*(8), 1638–1647. https://doi.org/10.1039/d4dd00093e

7. Gallarati, S., van Gerwen, P., **Laplaza**, **R.**, Brey, L., Makaveev, A., & Corminboeuf, C. (2024). A genetic optimization strategy with generality in asymmetric organocatalysis as a primary target. *Chem. Sci.*, *15*(10), 3640–3660. https://doi.org/10.1039/d3sc06208b

8. Blaskovits, J. T., **Laplaza**, **R.**, Vela, S., & Corminboeuf, C. (2023). Data-driven discovery of organic electronic materials enabled by hybrid top-down/bottom-up design. *Adv. Mater.*, *36*(2), 2305602. https://doi.org/10.1002/adma.202305602

9. van Gerwen, P., Wodrich, M. D., **Laplaza**, **R.**, & Corminboeuf, C. (2023). Reply to comment on 'physics-based representations for machine learning properties of chemical reactions'. *Mach. Learn.: Sci. Technol.*, *4*(4), 048002. https://doi.org/10.1088/2632-2153/acee43

10. Novoa, T., **Laplaza**, **R.**, Peccati, F., Fuster, F., & Contreras-García, J. (2023). The NCIWEB server: A novel implementation of the noncovalent interactions index for biomolecular systems. *J. Chem. Inf. Model.*, *63*(15), 4483–4489. https://doi.org/10.1021/acs.jcim.3c00271

11. Wodrich, M. D., **Laplaza**, **R.**, Cramer, N., Reiher, M., & Corminboeuf, C. (2023). Toward in silico catalyst optimization. *CHIMIA*, *77*(3), 139. https://doi.org/10.2533/chimia.2023.139

12. Gallarati, S., Gerwen, P. V., Schoepfer, A. A., **Laplaza**, **R.**, & Corminboeuf, C. (2023). Genetic algorithms for the discovery of homogeneous catalysts. *CHIMIA*, *77*(1/2), 39. https://doi.org/10.2533/chimia.2023.39

13. Wieduwilt, E. K., Boto, R. A., Macetti, G., **Laplaza**, **R.**, Contreras-García, J., & Genoni, A. (2023). Extracting quantitative information at quantum mechanical level from noncovalent interaction index analyses. *J. Chem. Theory Comput.*, *19*(3), 1063–1079. https://doi.org/10.1021/acs.jctc.2c01092

14. **Laplaza**, **R.**, Das, S., Wodrich, M. D., & Corminboeuf, C. (2022). Constructing and interpreting volcano plots and activity maps to navigate homogeneous catalyst landscapes. *Nat. Protoc.*, *17*(11), 2550–2569. https://doi.org/10.1038/s41596-022-00726-2

15. Vela, S., **Laplaza**, **R.**, Cho, Y., & Corminboeuf, C. (2022). Cell2mol: Encoding chemistry to interpret crystallographic data. *npj Comput. Mater.*, *8*(1), 188. https://doi.org/10.1038/s41524-022-00874-9

16. Das, S., **Laplaza**, **R.**, Blaskovits, J. T., & Corminboeuf, C. (2022). Mapping active site geometry to activity in immobilized frustrated Lewis pair catalysts. *Angew. Chem. Int. Ed.*, *134*(32). https://doi.org/10.1002/ange.202202727

17. Jurásková, V., Célerse, F., **Laplaza**, **R.**, & Corminboeuf, C. (2022). Assessing the persistence of chalcogen bonds in solution with neural network potentials. *J. Chem. Phys.*, *156*(15), 154112. https://doi.org/10.1063/5.0085153

18. **Laplaza**, **R.**, Gallarati, S., & Corminboeuf, C. (2022). Genetic optimization of homogeneous catalysts. *Chemistry–Methods*, *2*(6), e202100107. https://doi.org/10.1002/cmtd.202100107

19. Schwaller, P., Vaucher, A. C., **Laplaza**, **R.**, Bunne, C., Krause, A., Corminboeuf, C., & Laino, T. (2022). Machine intelligence for chemical reaction space. *WIREs Comput. Mol. Sci.*, *12*(5). https://doi.org/10.1002/wcms.1604

20. **Laplaza**, **R.**, Contreras-Garcia, J., Fuster, F., Volatron, F., & Chaquin, P. (2022). Dependence of hydrocarbon sigma CC bond strength on bond angles: The concepts of "inverted", "direct" and "superdirect" bonds. *Comput. Theor. Chem.*, *1207*, 113505. https://doi.org/10.1016/j.comptc.2021.113505

21. Gallarati, S., **Laplaza**, **R.**, & Corminboeuf, C. (2022). Harvesting the fragment-based nature of bifunctional organocatalysts to enhance their activity. *Org. Chem. Front.*, *9*(15), 4041–4051. https://doi.org/10.1039/d2qo00550f

22. Gallarati, S., van Gerwen, P., **Laplaza**, **R.**, Vela, S., Fabrizio, A., & Corminboeuf, C. (2022). OSCAR: An extensive repository of chemically and functionally diverse organocatalysts. *Chem. Sci.*, *13*(46), 13782–13794. https://doi.org/10.1039/d2sc04251g

23. Garner, M. H., **Laplaza**, **R.**, & Corminboeuf, C. (2022). Helical versus linear Jahn–Teller distortions in allene and spiropentadiene radical cations. *Phys. Chem. Chem. Phys.*, *24*(42), 26134–26143. https://doi.org/10.1039/d2cp03544h

24. Landeros-Rivera, B., Gallegos, M., Munarriz, J., **Laplaza**, **R.**, & Contreras-Garcia, J. (2022). New venues in electron density analysis. *Phys. Chem. Chem. Phys.*, *24*(36), 21538–21548. https://doi.org/10.1039/d2cp01517j

25. **Laplaza**, **R.**, Sobez, J.-G., Wodrich, M. D., Reiher, M., & Corminboeuf, C. (2022). The (not so) simple prediction of enantioselectivity – a pipeline for high-fidelity computations. *Chem. Sci.*, *13*(23), 6858–6864. https://doi.org/10.1039/d2sc01714h

26 Romero-Tamayo, S., **Laplaza**, **R.**, Velazquez-Campoy, A., Villanueva, R., Medina, M., & Ferreira, P. (2021). W196 and the β-hairpin motif modulate the redox switch of conformation and the biomolecular interaction network of the apoptosis-inducing factor. *Oxid. Med. Cell. Longev.*, *2021*, 1–19. https://doi.org/10.1155/2021/6673661

27 Gallarati, S., Fabregat, R., **Laplaza**, **R.**, Bhattacharjee, S., Wodrich, M. D., & Corminboeuf, C. (2021). Reaction-based machine learning representations for predicting the enantioselectivity of organocatalysts. *Chem. Sci.*, *12*(20), 6879–6889. https://doi.org/10.1039/d1sc00482d

28 **Laplaza**, **R.**, Cárdenas, C., Chaquin, P., Contreras-García, J., & Ayers, P. W. (2020). Orbital energies and nuclear forces in <scp>DFT</scp> : Interpretation and validation. *J. Comput. Chem.*, *42*(5), 334–343. https://doi.org/10.1002/jcc.26459

29 **Laplaza**, **R.**, Peccati, F., A. Boto, R., Quan, C., Carbone, A., Piquemal, J.-P., Maday, Y., & Contreras-García, J. (2020). NCIPLOT and the analysis of noncovalent interactions using the reduced density gradient. *WIREs Comput. Mol. Sci.*, *11*(2).

30 Boto, R. A., Peccati, F., **Laplaza**, **R.**, Quan, C., Carbone, A., Piquemal, J.-P., Maday, Y., & Contreras-García, J. (2020). NCIPLOT4: Fast, robust, and quantitative analysis of noncovalent interactions. *J. Chem. Theory Comput.*, *16*(7), 4150–4158. https://doi.org/10.1021/acs.jctc.0c00063

31 **Laplaza**, **R.**, Contreras-Garcia, J., Fuster, F., Volatron, F., & Chaquin, P. (2020). The "Inverted bonds" revisited: Analysis of "In silico" models and of [1.1.1]Propellane by using orbital forces. *Chem. Eur. J.*, *26*(30), 6839–6845. https://doi.org/10.1002/chem.201904910

32 **Laplaza**, **R.**, Boto, R. A., Contreras-García, J., & Montero-Campillo, M. M. (2020). Steric clash in real space: Biphenyl revisited. *Phys. Chem. Chem. Phys.*, *22*(37), 21251–21256. https://doi.org/10.1039/d0cp03359f

33 **Laplaza**, **R.**, Polo, V., & Contreras-García, J. (2019a). A bond charge model ansatz for intrinsic bond energies: Application to C–C bonds. *J. Phys. Chem. A*, *124*(1), 176–184. https://doi.org/10.1021/acs.jpca.9b10251

34 Villanueva, R., Romero-Tamayo, S., **Laplaza**, **R.**, Martínez-Olivan, J., Velázquez-Campoy, A., Sancho, J., Ferreira, P., & Medina, M. (2019). Redox- and ligand binding-dependent conformational ensembles in the human apoptosis-inducing factor regulate its pro-life and cell death functions. *Antioxid. Redox Signal.*, *30*(18), 2013–2029. https://doi.org/10.1089/ars.2018.7658

35 Peccati, F., **Laplaza**, **R.**, & Contreras-García, J. (2019). Overcoming distrust in solid state simulations: Adding error bars to computational data. *J. Phys. Chem. C*, *123*(8), 4767–4772. https://doi.org/10.1021/acs.jpcc.8b10510

36 **Laplaza**, **R.**, Polo, V., & Contreras-García, J. (2019b). Localizing electron density errors in density functional theory. *Phys. Chem. Chem. Phys.*, *21*(37), 20927–20938. https://doi.org/10.1039/c9cp02806d

37 Munárriz, J., **Laplaza**, **R.**, Martín Pendás, A., & Contreras-García, J. (2019). A first step towards quantum energy potentials of electron pairs. *Phys. Chem. Chem. Phys.*, *21*(8), 4215–4223. https://doi.org/10.1039/c8cp07509c

38 Munárriz, J., **Laplaza**, **R.**, & Polo, V. (2018). A bonding evolution theory study on the catalytic noyori hydrogenation reaction. *Mol. Phys.*, *117*(9-12), 1315–1324. https://doi.org/10.1080/00268976.2018.1542168

39 Quero, J., Cabello, S., Fuertes, T., Mármol, I., **Laplaza**, **R.**, Polo, V., Gimeno, M. C., Rodriguez-Yoldi, M. J., & Cerrada, E. (2018). Proteasome versus thioredoxin reductase competition as possible biological targets in antitumor mixed thiolate-dithiocarbamate Gold(III) complexes. *Inorg. Chem.*, *57*(17), 10832–10845. https://doi.org/10.1021/acs.inorgchem.8b01464

40 Martínez-Júlvez, M., Goñi, G., Pérez-Amigot, D., **Laplaza**, **R.**, Ionescu, I., Petrocelli, S., Tondo, M., Sancho, J., Orellano, E., & Medina, M. (2017). Identification of inhibitors targeting ferredoxin-NADP+ reductase from the xanthomonas citri subsp. citri phytopathogenic bacteria. *Molecules*, *23*(1), 29. https://doi.org/10.3390/molecules23010029

Books and Chapters

1 **Laplaza**, **R.**, Munárriz, J., & Contreras-García, J. (2022). Chemical information. In *Conceptual density functional theory: Towards a new chemical reactivity theory* (pp. 349–374). Wiley. https://doi.org/10.1002/9783527829941.ch18

2 **Laplaza**, **R.**, Peccati, F., Arias-Olivares, D., & Contreras-García, J. (2021). 14 visualizing non-covalent interactions with NCIPLOT. In *Complementary bonding analysis* (pp. 353–378). De Gruyter. https://doi.org/10.1515/9783110660074-014

Congress Presentations

- Navigating Homogeneous Catalyst Landscapes — Oral contribution, 13^{th} *Congress on Electronic Structure: Principles and Applications (ESPA2024)*, Tarragona, Spain, 2024
- Navigating Molecular Catalyst Landscape with NaviCat — Oral contribution, *Chemical Compound Space Conference*, Heidelberg, Germany, 2024
- Tapping into Crystallographic Repositories with cell2mol — Poster, *The Path of Quantum Chemistry into the 21st Century*, Zurich, Switzerland, 2024
- Navigating Molecular Catalyst Landscape with NaviCat — Poster, *Chemical Concepts from Theory and Computation*, Lyon, France, 2023
- cell2mol: Unlocking Crystallographic Repositories for Computational Chemistry — Poster, *Bridging length scales with machine learning: from wavefunctions to thermodynamics*, Berlin, Germany, 2023
- NaviCat: Computational Tools to Navigate Molecular Catalyst Landscape — Poster, *12th WATOC Conference*, Vancouver, Canada, 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*, Online, 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.
- 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 (QCrOM2020)*, 2020.
- Best junior talk award, *Chemical Compound Space Conference*, 2024.

Other Merits (continued)

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 *Angew. Chem. Int. Ed.*, *Nat. Comm.*, *Mach. Learn.: Sci. Technol*, *J. Chem. Theory Comput.*, *Phys. Chem. Chem. Phys.*, *Digital Discovery* and other digital and computational chemistry journals.

Invited seminars

Institut de Sciences Analytiques	*"Machine Learning and Generative Models: From Structure to Properties and Back"*, January 2024.
IBM Research Zurich	*"NaviCat: Computational Tools to Navigate Molecular Catalyst Landscapes"*, July 2022.