Lionel Zoubritzky
(Post-doctoral Research Fellow)

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RESEARCH INTERESTS

Numerical simulation of CO_2 reduction

- Frustrated Lewis Pairs
- XAS analysis of heterogeneous catalysts
- Photocatalysis

EDUCATIONAL BACKGROUND

2025-current	Post-doctoral Research Fellow Collège de France, Paris, France.
2021-2024	PhD in Numerical Chemistry Chimie ParisTech – PSL, Paris, France and Air Liquide, Les Loges-en-Josas, France.
2016-2021	Diploma with a double major in computer science and chemistry École Normale Supérieure – PSL, Paris, France.
2019-2021	Master in Chemistry, minor in Materials Science École Normale Supérieure – PSL and Sorbonne Université, Paris, France.
2018-2019	MPhil in Advanced Computer Science University of Cambridge, Cambridge, UK
2016-2018	L3 and M1 in Computer Science École Normale Supérieure – PSL, Paris, France.

SUMMARY

I am a theoretical chemist specialized on the numerical simulation of gas adsorption and reactivity. During my PhD, I designed new methodologies for studying the adsorption of small gases, such as CO_2, on zeolites and MOFs. In particular, I developed an open-source tool called “CrystalNets”, freely available to the scientific community, which identifies the topology of crystalline materials. My current research focuses on the conversion of CO_2 into molecules of greater economic interest such as formic

acid or methane. I computationally study several reduction pathways through photocatalysis and thermal catalysis, either supported by metallic nanoparticles or by non-metallic Frustrated Lewis Pairs (FLPs), in both homogeneous and heterogeneous settings.

PUBLICATIONS

2025

- Penas-Hidalgo, F., **Zoubritzky, L.**, Solé-Daura, A. & Mellot-Draznieks, C. Structure–Activity Relationships in H2 Splitting by Frustrated Lewis Pairs: From Fundamental Understanding to Data-Driven Design Rules. In submission.
- **Zoubritzky, L.**, & Coudert, F.-X. CrystalNets: a web app for topology determination of crystalline structures. In submission.
- **Zoubritzky, L.**, & Coudert, F.-X. (2025). Large-scale characterization of chemical bonding and topology in the Materials Project database. Chemistry of Materials, 37(9), 3137-3146.
- Zhao, G., Brabson, L. M., Chheda, S., Huang, J., Kim, H., Liu, K., Mochida, K., Pham, T. D., Prerna, Terrones, G. G., Yoon, S., **Zoubritzky, L.**, Coudert, F.-X., Haranczyk, M., Kulik, H. J., Moosavi, S. M., Sholl, D. S., Siepmann, J. I., Snurr, R. Q. & Chung, Y. G. (2025). CoRE MOF DB: A curated experimental metal-organic framework database with machine-learned properties for integrated material-process screening. Matter, 8(6).

2022

- **Zoubritzky, L.**, & Coudert, F. X. (2022). CrystalNets.jl: Identification and Classification of Crystal Topologies. SciPost Chemistry, 1(005).
- **Zoubritzky, L.** & Bunel, L. (2022). Chimiophobie ? L'évolution du rejet de la chimie par la société. CultureSciences-Chimie.

2021

- Ainsworth, S., **Zoubritzky, L.**, Mycroft, A., & Jones, T. M. (2021, February). Paradox: Eliminating voltage margins via heterogeneous fault tolerance. In 2021 IEEE International Symposium of High-Performance Computer Architecture (HPCA) (pp. 520-532). IEEE.

2018

- Bezanson, J., Chen, J., Chung, B., Karpinski, S., Shah, V. B., Vitek, J., & **Zoubritzky, L.** (2018). Julia: Dynamism and performance reconciled by design. Proceedings of the ACM on Programming Languages, 2(OOPSLA), 1-23.
- **Zoubritzky, L.**, & Schmitt, A. (2018). HOcore en HOcore. Journées Francophones des Langages Applicatifs, 77.