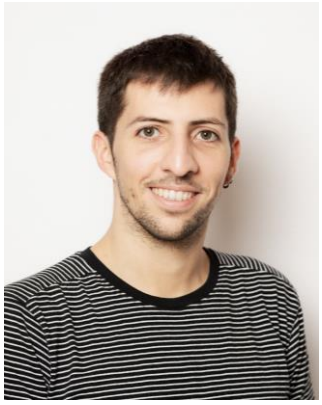
Dr Albert Solé-Daura
(Post-doctoral Research Fellow)



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RESEARCH INTERESTS

Computational catalysis and molecular dynamics

- Structure and reactivity of polyoxometalates and metal-organic frameworks
- Molecular and supramolecular catalysis
- Reaction mechanisms and catalyst design
- Self-assembly and host-guest interactions
- Proton and electron-transfer reactions
- MD methods and enhanced-sampling techniques

SUMMARY

My research activities mainly concern the application of computational methods to the study of the electronic properties and reactivity of polyoxometalates (POMs) and metal-organic frameworks (MOFs) for their application in catalysis. During my doctoral studies, I also acquired extensive experience in modelling dynamic properties of inorganic clusters such as POMs in solution by means of atomistic Molecular Dynamics simulations, including their speciation, self-assembly processes inducing agglomeration, or host-guest interactions responsible for their specific binding to other bodies such as proteins. Besides, I am highly interested in the computational modelling of chemical reactivity accounting for an explicit and dynamic description of the environment, as well as in the study of reactions that involve proton and electron-transfer processes.

PUBLICATIONS

2021

- "Understanding the Heterogeneous Photocatalytic Reduction of CO_2 with Heterometallic Molybdenum(V)-Phosphate Polyoxometalates in Aqueous Media" Benseghir, Y.; **Solé-Daura, A.**; Mialane, P.; Marrot, J.; Dalecky, L.; Gomez-Mingot, M.; Fontecave, M.; Mellot-Draznieks, C.; Dolbecq, A. (*submitted*)
- "Activation of H_2O_2 over Zr(IV). Insights from Model Studies on Zr-Monosubstituted Lindqvist Tungstates" Maksimchuk, N. V.; Evtushok, V. Y.; Zalomaeva, O. V.; Maksimov, G. M.; Ivanchikova, I. D.; Chesalov, Y. A.; Eltsov, I. V.; Abramov, P. A.; Glazneva, T. S.; Yanshole, V. V.; Kholdeeva, O. A.; Errington, R. J.; **Solé-Daura, A.**; Poblet, J. M.; Carbó, J. J. ***ACS Catal.*** 2021, *11*, 10589-10603.
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Polyoxometalates" Zhang, T.; **Solé-Daura, A.**; Fouilloux, H.; Poblet, J. M.; Proust, A.; Carbó, J. J.; Guillemot, G. ***ChemCatChem*** 2021, *13,* 1220-1229*.*

- "*Discovery and supramolecular interactions of neutral palladium-oxo clusters Pd_{16} and Pd_{24}*" Bhattacharya, S.; Basu, U.; Haouas, M.; Su, P.; Espenship, M. F.; Wang, F.; **Solé-Daura, A.**; Taffa, D. H.; Wark, M.; Poblet, J. M.; Laskin, J.; Cadot, E.; Kortz, U. ***Angew. Chem. Int. Ed.*** 2021, *60*, 3632-3639.
- "Peptide Hydrolysis by Metal-(Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects" Gantulga, N.; **Solé-Daura, A.**; Ricart, J. M.; Carbó, J. J. ***Inorg. Chem.*** 2021*, 60*, 807-815.

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- "Structure-Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins" **Solé-Daura, A.**; Poblet, J. M.; Carbó, J. J. ***Chem. Eur. J.*** 2020, *26*, 5799–5809 (frontispiece).
- "Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts" **Solé-Daura, A.**; Zhang, T.; Fouilloux, H.; Robert, C.; Thomas, C. M.; Chamoreau, L.-M.; Carbó, J. J. Proust, A.; Guillemot, G.; Poblet, J. M. ***ACS Catal.*** 2020, *10*, 4737–4750 (inside cover).
- "Chemical Reactions of Cationic Metallofullerenes: An Alternative Route for Exohedral Functionalization" Hu, Y.; **Solé-Daura, A.**; Yao, Y.-R.; Liu, X.; Liu, S.; Yu, A.; Peng, P.; Poblet, J. M.; Rodríguez-Fortea, A.; Echegoyen, L.; Li, F.-F. ***Chem. Eur. J.*** 2020, *26*, 1748–1753.

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- "Polyoxometalates as alternative Mo precursors for methane dehydroaromatization on Mo/ZSM-5 and Mo/MCM-22 catalysts" Julian, I.; Hueso, J. L.; Lara, N.; **Solé-Daura, A.**; Poblet, J. M.; Mitchell, S. G.; Mallada, R.; Santamaria, J. ***Catal. Sci. Technol.*** 2019, *9*, 5927–5942.
- "Peroxo-Cerium(IV)-Containing Polyoxometalates: $[Ce^{IV}_6(O_2)_9(GeW_{10}O_{37})_3]^{24-}$, a Recyclable Homogeneous Oxidation Catalyst" Qasim, H. M.; Ayass, W. W.; Donfack, P.; Mougharbel, A. S.; Bhattacharya, S.; Nisar, T.; Balster, T.; **Solé-Daura, A.**; Römer, I.; Goura, J.; Materny, A.; Wagner, V.; Poblet, J. M.; Bassil, B. S.; Kortz, U. ***Inorg. Chem.*** 2019, *58*, 11300–11307.
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- "How Does the Redox State of Polyoxovanadates Influence the Collective Behavior in Solution? A Case Study with $[I@V_{18}O_{42}]^{q-}$ (q = 3, 5, 7, 11, and 13)" **Solé-Daura, A.**; Notario-Estévez, A.; Carbó, J. J.; Poblet, J. M.; De Graaf, C.; Monakhov, K. Y.; López, X. ***Inorg. Chem.*** 2019, *58*, 3881–3894.

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- "Self-Assembly Study of Nanometric Spheres from Polyoxometalate-Phenylalanine Hybrids, an Experimental and Theoretical Approach" Nikoloudakis, E.; Karikis, K.; Laurans, M.; Kokotidou, C.; **Solé-Daura, A.**; Carbó, J. J.; Charisiadis, A.; Charalambidis, G.; Izzet, G.; Mitraki, A.; Douvas, A. M.; Poblet, J. M.; Proust, A.; Coutsolelos, A. G. ***Dalton Trans.*** 2018*, 47*, 6304–6313 (inside cover).

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- "Molecular Characteristics of a Mixed-Valence Polyoxovanadate $\{V^{IV/V}_{18}O_{42}\}$ in Solution and at the Liquid–Surface Interface" Linnenberg, O.; Moors, M.; **Solé-Daura, A.**; López, X.; Bäumer, C.; Kentzinger, E.; Pyckhout-Hintzen, W.; Monakhov, K. Y. ***J. Phys. Chem. C*** 2017, *121*, 10419–10429.
- "Core-Substituted Naphthalenediimides Anchored on BiVO4 for Visible Light-Driven Water Splitting" Hernández, S.; Ottone, C.; Proto, S.; Tolod, K.; Díaz de los Bernardos, M.; **Solé-Daura, A.**; Carbó, J. J.; Godard, C.; Castillón, S.; Russo, N.; Saracco, G.; Claver, C. ***Green Chem.*** 2017*, 19*, 2448–2462*.*

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