

Selected publications

1. "Complete σ^* Intramolecular Aromatic Hydroxylation Mechanism through O₂ Activation by a Macrocyclic Dinuclear Copper(I) Complex"

J. Am. Chem. Soc. **2008**, *130*, 17710-17711.

Poater, A.; Ribas, X.; Cavallo, L.; Llobet, A.; Sola, M.

2. "Oxygen-oxygen bond formation by the Ru-Hbpp water oxidation catalyst occurs solely via an intramolecular reaction pathway"

J. Am. Chem. Soc. **2009**, *131*, 2768-2769.

Romain, S.; Bozoglian, F.; Sala, X.; Llobet, A.

3. "Water oxidation catalysts based on transition metal complexes"

Angew. Chem. Int. Ed. **2009**, *48*, 2842-2852.

Sala, X.; Romero, I.; Rodríguez, R.; Escriche, L.; Llobet, A.

4. "The Ru-Hbpp Water Oxidation Catalyst"

J. Am. Chem. Soc. **2009**, *131*, 15176-15187.

Bozoglian, F.; Romain, S.; Ertem, M. Z.; Todorova, T. K.; Sens, C.; Mola, J.; Rodríguez, M.; Cramer, C. J.;

Gagliardi, L.; Llobet, A. et al.

5. "Water Oxidation at a Tetra-ruthenate Core stabilized by Polyoxometalate Ligands: Experimental and Computational Evidence to trace the Competent Intermediates"

J. Am. Chem. Soc. **2009**, *131*, 16051-16053.

Sartorel, A.; Miro, P.; Salvadori, E.; Romain, S.; Carraro, M.; Scorrano, G.; Di Valentin, M.; Llobet, A.; Bo, C.; Bonchio, M.

6. "Oxygen-Oxygen Bond Formation Pathways Promoted by Ru Complexes"

Acc. Chem. Res. **2009**, *42*, 1944-1953.

Romain, S.; Vigara, L.; Llobet, A.

7. "Facile C-H bond cleavage via a proton coupled electron transfer involving a C-H...Cull interaction".

J. Am. Chem. Soc. **2010**, *132*, 12299-12306.

Ribas, X.; Calle, C.; Poater, A.; Casitas, A.; Gomez, L.; Xifra, R.; Parella, T.; Benet-Buchholz, J.; Schweiger, A.; Mitrikas, G.; Sola, M.; Llobet, A.; Stack, T. D. P.

8. "The cis-[Ru^{II}(bpy)₂(H₂O)₂]²⁺ Water-Oxidation Catalyst Revisited"

Angew. Chem. Int. Ed. **2010**, *49*, 7745-7747.

Sala, X.; Ertem, M. Z.; Vigara, L.; Todorova, T. K.; Chen, W.; Rocha, R. C.; Cramer, C. J.; Gagliardi, L.; Llobet, A.

9. "Water Oxidation in the Context of the Energy Challenge: Tailored Transition-Metal Catalysts for Oxygen-Oxygen Bond Formation".

Angew. Chem. Int. Ed. **2011**, *50*, A30-A33.

Llobet, A.; Meyer, F.

10. "A Molecular Ruthenium Catalyst with the Water-Oxidation Activity Comparable to that of Photosystem II"

Nat. Chem. **2012**, *4*, 418-423.

Duan, L.; Bozoglian, F.; Mandal, S.; Stewart, B.; Privalov, T.; Llobet, A. Sun, L.

11. "Ligand Geometry Directs O-O Bond Formation Pathway in New trans-RuHbpp Based Water Oxidation Catalyst"
Angew. Chem. Int. Ed. **2012**, *51*, 5967-5970.
Maji, S.; Vigara, L.; Cottone, F.; Bozoglian, F.; Benet-Buchholz, J.; Llobet, A.
12. "Catalytic Four-Electron Reduction of Dioxygen via Rate-Determining Proton-Coupled Electron Transfer to a Dinuclear Cobalt- μ -1,2-Peroxo Complex"
J. Am. Chem. Soc. **2012**, *134*, 9906-9909.
Fukuzumi, S.; Mandal, S.; Mase, K.; Ohkubo, K.; Park, H.; Benet-Buchholz, J.; Nam, W.; Llobet, A.
13. "Synthesis, Electronic Structure and Magnetism of $[\text{Ni}(\text{6-Mes})_2]^+$: A Two-Coordinate Nickel(I) Complex Stabilized by Bulky N-Heterocyclic Carbenes"
J. Am. Chem. Soc. **2013**, *135*, 13640-13643.
Poulten, R. C.; Page, M. J.; Algarra, A. G.; Le Roy, J. J.; Lopez, I.; Carter, E.; Llobet, A.; Macgregor, S. A.; Mahon, M. F.; Murphy, D. M.; Murugesu, M.; Whittlesey, M. K.
14. "Protonation Equilibrium and Hydrogen Production by a Dinuclear Cobalt- μ -Hydride Complex Reduced by Cobaltocene with Trifluoroacetic Acid"
J. Am. Chem. Soc. **2013**, *135*, 15294-15297.
Mandal, S.; Shikano, S.; Yamada, Y.; Lee, Y.-M.; Nam, W.; Llobet, A.; Fukuzumi, S.
15. "A Self-improved Water Oxidation Catalyst; Is One Site Really Enough?"
Angew. Chem. Int. Ed. **2014**, *53*, 205-210.
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16. "Molecular Water Oxidation Mechanisms Followed by Transition Metals: State of the Art"
Acc. Chem. Res., **2014**, *47*, 504-516.
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17. "New Powerful and Oxidatively Rugged Dinuclear Ru WOCs: Control of Mechanistic Pathways by Tailored Ligand Design"
J. Am. Chem. Soc. **2014**, *136*, 24-27.
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18. "Molecular Artificial Photosynthesis"
Chem. Soc. Rev., **2014**, *43*, 7501-7519.
Berardi, S.; Drouet, S.; Francàs, L.; Gimbert-Suriñach, C.; Guttentag, M.; Richmond, C.; Stoll, T.; Llobet, A.
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J. Am. Chem. Soc. **2014**, *136*, 7655-7661.
Gimbert-Surinach, C.; Albero, J.; Stoll, T.; Fortage, J.; Collomb, M.-N.; Deronzier, A.; Palomares, E.; Llobet, A.
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J. Am. Chem. Soc. **2015**, *137*, 6758-6761.
Garrido-Barros, P.; Funes-Ardoiz, I.; Drouet, S.; Benet-Buchholz, J.; Maseras, F.; Llobet, A.
21. "Intramolecular proton transfer boosts water oxidation catalyzed by a Ru complex"
J. Am. Chem. Soc. **2015**, *137*, 10786-10795.
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22. "Tracking the Structural and Electronic Configurations of a Cobalt Proton Reduction Catalyst in Water".
J. Am. Chem. Soc. **2016**, *138*, 10586-10596.
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23. "A Million Turnover Molecular Anode for Catalytic Water Oxidation."
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J. Am. Chem. Soc. **2017**, *139*, 11345-11348.
Matheu, R.; Moreno-Hernandez, I. A.; Sala, X.; Gray, H. B.; Brunschwig, B. S.; Llobet, A.; Lewis, N. S.
26. "Electronic π -delocalization Boosts Catalytic Water Oxidation by Cu(II) Molecular Catalysts Heterogenized on Graphene Sheets."
J. Am. Chem. Soc. **2017**, *139*, 12907-12910.
Garrido-Barros, P.; Gimbert-Suriñach, C.; Moonshiram, D.; Picon, A.; Monge, P.; Batista, V. S.; Llobet, A.
27. "The development of molecular water oxidation catalysts"
Matheu, R.; Garrido-Barros, P.; Gil-Sepulcre, M.; Ertem, M. Z.; Sala, X.; Gimbert-Suriñach, C.; Llobet, A.
Nat. Rev. Chem. **2019**, *3*, 331-341.
28. "Seven Coordinated Molecular Ruthenium–Water Oxidation Catalysts: A Coordination Chemistry Journey"
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Chem. Rev. **2019**, *119*, 3453–3471.
29. "Second Coordination Sphere Effects in an Evolved Ru Complex Based on a Highly Adaptable Ligand Results in Rapid Water Oxidation Catalysis"
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J. Am. Chem. Soc. **2020**, *142*, 5068-5077.

Book

'Molecular Water Oxidation Catalysis: A Key Topic for New Sustainable Energy Conversion Schemes'.

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