

# Dr. Antoine Simonneau

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born March 6, 1985, French nationality

marital status: under the regime of the French solidarity civil pact

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## CURRENT SITUATION

**Chargé de Recherche Classe Normale (Junior Researcher)**, Laboratoire de Chimie de Coordination (LCC), Centre National de la Recherche Scientifique (CNRS) and Université Paul Sabatier (UPS) - Toulouse III, since **Nov. 2015**. Team leader since **2019**.

**Research interests:** *Activation of small molecules (N<sub>2</sub>, H<sub>2</sub>, CO<sub>2</sub>) and strong bonds (C–F) through cooperative methods involving reactive organometallic, inorganic and main-group molecular species.*

## PREVIOUS EXPERIENCE

**Oct. 2012–  
Jul. 2015**      **Postdoctoral researcher** in the group of Prof. M. OESTREICH (Technische Universität, Berlin), as an **Alexander von Humboldt postdoctoral fellow** between **Feb. 2014** and **Jul. 2015**.

Project: *Development of transfer hydrosilylation methodologies and reactivity of strong main group electrophiles*

**Feb. 2012–  
Jun. 2012**      **Postdoctoral researcher** in the group of Dr. C. AUBERT and Prof. L. FENSTERBANK (Institut Parisien de Chimie Moléculaire, Université Pierre et Marie Curie, Paris, France).

Project: *Chiral phosphate ligands for atroposelective, rhodium-catalyzed [2 + 2 + 2] cycloadditions.*

## EDUCATION

**Jul. 2020**      **Habilitation, University of Toulouse.** Thesis: *"Dinitrogen transformation: towards molecular solutions based on zero-valent group 6 complexes"*.

**Oct. 2008–  
Dec. 2011**      **Ph.D. in Organic Chemistry, with highest honors**, in the group of Profs. M. MALACRIA and L. FENSTERBANK (Institut Parisien de Chimie Moléculaire, Sorbonne Université (formerly Université Pierre et Marie Curie), Paris, France), **Springer Thesis Prize 2014**.

**Thesis:** *Gold-catalyzed Cycloisomerization Reactions through Activation of Alkynes: New Developments and Mechanistic Studies.* Published by Springer International Publishing Switzerland.

Ph.D. thesis defended the **9<sup>th</sup> December 2011**, issued **11<sup>th</sup> January 2012**.

**Sep. 2007–  
Jul. 2008**      **Master of Science in Organic and Bioorganic Chemistry, with honors** (Université Pierre et Marie Curie, Paris). M. Sc. thesis in the group of Prof. G. JAUQUEN and Dr. F. LEBIDEAU (École Nationale Supérieure de Chimie de Paris). Project: *Diastereoselective synthesis of octahedral carbonyl complexes of rhenium.*

**Sep. 2005–  
Jul. 2008**      **Chemical Engineering degree** (french "Diplôme d'Ingénieur") of the École Nationale Supérieure de Chimie de Paris.

## AWARDS & FELLOWSHIPS

**Jun. 2024**      **Young Researcher Award of the Coordination Chemistry Division of the French chemical Society.**

**Feb. 2022**      **Young Investigator Award of the Chemistry Institute of Toulouse (ICT).** 1.5 k€ travel grant awarding talented early-career chemists from laboratories based in Toulouse.

**Aug. 2017**      **ERC Starting Grant.** *The European Research Council selects and funds the very best, creative researchers of any nationality and age, to run projects based in Europe. ERC Starting Grants are awarded to researchers of any nationality with two to seven years of experience since completion of the PhD and a scientific track record showing great promise.*

**Nov. 2013**      **Alexander von Humboldt Research Fellowship.** *Through the Humboldt Research Fellowship, the Alexander von Humboldt Foundation sponsors researchers with above-average qualifications from across the globe.*

**Feb. 2014**      **Springer Thesis Prize.** *Internationally top-ranked research institutes select their best thesis annually for publication in this series. Nominated and endorsed by two recognized specialists, each thesis is chosen for its scientific excellence and impact on research.*

## INSTITUTIONAL RESPONSIBILITIES

since 2023	Member of the LCC "Sustainability" working group.
2020–2022	Member of the LCC "Website" working group.
Since March 2019	Co-supervisor of the Small Molecule Activation (SMAC) Team, Laboratoire de Chimie de Coordination. Supervision shared with S. Bontemps.

## SUPERVISION AND EVALUATION OF RESEARCH TRAINING

2017–2020	Anaïs Coffinet, PhD (Univ. Toulouse), 100% supervision rate.
2018–2021	Dr. David Specklin, postdoctoral associate.
2018–2022	Amal Bouammali, PhD (Univ. Toulouse), 100% supervision rate.
2019–2023	Quentin Le Dé, PhD (Univ. Toulouse), 100% supervision rate.
2020–2024	Marie-Christine Boegli, PhD (Univ. Toulouse), 100% supervision rate.
Dec. 2020	PhD defense committee of Lydia Merakeb (LEM, Univ. Paris-Cité), examiner.
2020–2022	Dr. Nicolas Queyriaux, postdoctoral associate.
2020–2024	Sara Bonfante, PhD (Univ. Toulouse and Univ. of York), co-supervision (50%) with Dr. John Slattery.
2021–2025	Arno Estival, PhD (Univ. Toulouse), co-supervision (50%) with Dr. Mary Grellier, LCC-University of Toulouse.
2023–2025	Dr. Léon Escomel, postdoctoral associate.
Nov. 2023	PhD defense committee of Vincent Wowk (i-CLeHS, Chimie ParisTech), reviewer.
2024	Luis Blancarte, PhD (Autonomous National University of Mexico), research stay.
Jan. 2024	PhD defense committee of Mathieu Pascaretti (URCOM, Univ. Le Havre), reviewer.
Sep. 2024	PhD defense committee of Francesco Crisanti (LEM, Sorbonne Univ.), examiner.
2024–	Quentin Lepeintre, PhD (Univ. Toulouse), co-supervision (50%) with Prof. M. Drover, Western University (Canada).
Jan. 2025	PhD defense committee of Victor Monnot (CEMCA, Univ. Brest), reviewer.
since 2015	Supervision of 15 undergraduate internships (12 University of Toulouse, 1 University of Nantes, 1 ENSCM, 1 MITACS fellow from University of Montreal).

## TEACHING ACTIVITIES

Jun. 2022	2 <sup>nd</sup> C@T Summer School, École des Mines D'Albi. 1.5 h teaching on homogeneous nitrogen fixation.
Oct. 2020	CCIMC Core Course (LCC, Toulouse). 2 h teaching on homogeneous nitrogen fixation for the graduate students of the European Joint Doctorate program CCIMC.
Feb. 2019	XXXIX <sup>th</sup> Summer School of the Chemistry Department of the Federal University of São Carlos (UFSCar), Brazil under the theme "Chemistry and the Quality of Life". 9 h teaching on small molecules activation (homogeneous, photo- and electro-catalysis) related to energy transition and climate change. Graduate and undergraduate level. Title of the course: <i>Can Small Molecules Play A Role In Improving Quality Of Life ? Answers provided by current molecular chemistry.</i>
since 2016	Supervisor and jury for the chemical research project of the 1 <sup>st</sup> and 3 <sup>rd</sup> year bachelor students. Université Paul Sabatier, Toulouse, France.
Feb. 2009– Jul. 2011	Teaching assistant, practical courses of organic synthesis, bachelor level (250 hours). Institut Parisien de Chimie Moléculaire, Université Pierre et Marie Curie, Paris, France.

## EDITORIAL AND PEER-REVIEWING ACTIVITIES

2024–2025	Member of the Early Career Advisory Board of Inorg. Chem. Front. (RSC)
2023–2024	Member of the Early Career Advisory Board of JACS Au (ACS)
since 2016	>30 reviews for the following journals (please refer to my <a href="#">ORCID profile</a> )
	Angew. Chem Int. Ed.                      J. Am. Chem. Soc.                      Chem. Sci.
	Chem. Eur. J.                                  Chem. Asian J.                              Chem. Commun.
	Inorg. Chem.                                  Dalton Trans.                              Eur. J. Inorg. Chem.
	Inorg. Chem. Front.                        Nat. Commun.                              Science Advances

## EXPERT ASSESSMENTS FOR FUNDING AGENCIES

2024	Review for the UP-Squared program, Université de Poitiers
2022	2 reviews for the French National Research Agency
2021	Review for the French National Research Agency
2021	Review for the Dutch NWO Agency
2020	Review for the French National Research Agency

## ORGANIZATIONAL ACTIVITIES

2023–2024	<b>Member of the Organizing Committee of the GECOM-CONCOORD colloquium — Logistics &amp; Sponsors crew</b> , 20-24 May 2024, Ax-les-Thermes, France.
2020	<b>Member of the Organizing Committee of the online colloquium “Cutting-edge Homogeneous Catalysis” (CEHC-1)</b> , 4–6 May 2021, Toulouse, France.
2019–2020	<b>Member of the Organizing Committee of the European Colloquium on Inorganic Reaction Mechanisms (ECIRM)</b> , 12–15 July 2020, Toulouse, France (cancelled).

## PROFESSIONAL TRAINING

2024	<b>MOOC “Understanding Intellectual Property”</b> (8 h) from the French National Institute for Intellectual Property (INPI).
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## OUTREACH ACTIVITIES

2018–2019	<b>Welcome of high school students from “Lycée Toulouse-Lautrec” for a scientific project.</b> Supervision of glove-box experiments and reporting in a presentation.
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## FUNDING

2025–2026	<b>EMERGENCE @CNRS Chimie grant.</b> Covered 18-month postdoc salary + 15 k€.
2024–2027	<b>Doctoral fellowship of the France-Canada Research Fund - French Ministry of research and Higher Education.</b> Covered the salary of a PhD student over 3 years. <u>Co-principal investigator</u> .
2024–2026	<b>France-Canada Research Fund.</b> CA\$ 15 000 covering mobility expenses.
2024	<b>INFRANALYTICS Project.</b> Covered 15 days of NMR measurement at high field (800 and 1200 MHz). Solid state analysis of molecular molybdenum hydrides. <u>Principal Investigator</u> .
2022–2027	<b>International Research Project granted by the CNRS.</b> Funds researchers and student exchange in the frame of a collaborative research project between the LCC and the National Autonomous University of Mexico (UNAM). Coordinated by P. Lacroix (LCC) and Norberto Farfán (UNAM). Funded a stay at the UNAM (June 7–12 2022), and a 6-months research stay for a Mexican student.
2022–2026	<b>French National Research Agency (ANR) collaborative research grant.</b> Public funding for fundamental research. Project “PUNCh”, coordinated by M. Gennari, DCM, University of Grenoble-Alpes • 154 k€.
2021–2024	<b>Green Hydrogen grant.</b> Public funding for research on hydrogen and its applications. Project “CataLOHC”. <u>Principal Investigator</u> • 76 k€.
2020–2024	<b>International Training Network “CCIMC”.</b> European Joint Doctorate Program funded by the Marie Skłodowska-Curie Actions coordinated by R. Poli and A.-M. Caminade (LCC). Funded a joint Ph.D. fellowship and research costs. Partnering entity: Department of Chemistry of the University of York.
2018–2023	<b>ERC Starting Grant.</b> Covered among others salaries for 3 Ph.D. and 2 postdocs, equipment, travel and consumables. <u>Principal Investigator</u> • 1.5 M€.
2017–2020	<b>Doctoral fellowship of the French Ministry of research and Higher Education.</b> Covered the salary of a PhD student over 3 years.
2015–2017	<b>“Nouveaux Entrants” fellowship.</b> Seed money provided by the Université Fédérale Toulouse Midi-Pyrénées to help settlement of young researchers. <u>Principal Investigator</u> • 14 k€.
2014–2015	<b>Alexander von Humboldt Research Fellowship.</b> Covered salary and research costs for 18 months.
2017	<b>AAPG ANR JCJC</b> , project “MIDIFUNK” — PI, <b>not funded</b> .
2019	<b>International Emerging Action</b> , PI with Prof. C. Gruenwaldt (Univ. Sao Carlos, Brazil), <b>not funded</b> .
2023	<b>ERC Call “Proof-of-Concept”</b> , project HYDRa — PI, <b>not funded</b> (Seal of Excellence obtained).
2024	<b>AAPG ANR PRC</b> , project “MnN’s” — PI, <b>not funded</b> .
2024	<b>AAPG ANR PRC</b> , project “MimPhos” — partner, <b>not funded</b> .
2024	<b>ERC Call “Proof-of-Concept”</b> , project HYDRa — PI, <b>not funded</b> (Seal of Excellence obtained).

Peer-reviewed journals – Independent career

47. **Synthesis and Characterization of Heptacoordinated Molybdenum(II) Complexes Supported with 2,6-Bis(pyrazol-3-yl)pyridine (bpp) Ligands**, A. Estival, L. E. Blancarte, L. Pinto, R. Pointis, N. Galas, A. Sournia-Saquet, L. Vendier, R. Santillan, N. Farfán, J.-B. Sortais, M. Grellier and A. Simonneau,\* submitted.
46. **Bio-Inspired Thiolate-Fell-Hydrazine Adduct Towards Iron-Mediated C-N Bond Formation**, I. Cassandrini, C. Philouze, [A. Simonneau](#), C. Duboc and M. Gennari,\* in revision.
45. **Zirconium-Mediated Carbon-Fluorine Bond Functionalisation Through Cyclohexyne "Umpolung"**, S. Bonfante, T. F. N. Tanner, C. Lorber,\* J. M. Lynam,\* [A. Simonneau](#)\* and J. M. Slattery,\* in revision.
44. **Reactivity of Metal Hydrides with CO<sub>2</sub>: Going Beyond Formate with a High-Valent Cationic Pentahydride Mo(VI) Complex**, N. Queyriaux,\* J. J. Cabrera-Trujillo, N. Durvin, L. Vendier, K. Miqueu\* and [A. Simonneau](#)\*, *Chem. Sci.* **2024**, DOI: 10.1039/D4SC04345F.
43. **Low-valent Group 6 Metals/Al(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> Donor-Acceptor Systems for CO<sub>2</sub> Activation and Cleavage**, L. Escomel, Q. Le Dé, M. Benonie, L. Vendier and [A. Simonneau](#)\*, *Chem. Commun.*, **2024**, 60, 13235-13238.
42. **Coordination of Al(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> vs B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> on Group 6 End-On Dinitrogen Complexes: Chemical and Structural Divergences**, L. Escomel, F. Martins, L. Vendier, A. Coffinet, N. Queyriaux, V. Krewald\* and [A. Simonneau](#)\*, *Chem. Sci.* **2024**, 15, 11321-11336.
41. **Seven-coordinate Group 6 Metal Hydrides Obtained by H<sub>2</sub> Activation at B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> Adducts of N<sub>2</sub> Complexes: Frustrated Lewis Pair-type Reactivity of the B–N linkage**, M.-C. Boegli, A. Coffinet, C. Bijani and [A. Simonneau](#)\*, *Chem. Asian J.* **2024**, 19, e202400451.
40. **Nitrogen Fixation by Manganese Complexes – Waiting for the Rush? (Concept)** Q. Le Dé, D. A. Valyaev\* and [A. Simonneau](#)\*, *Chem. Eur J.* **2024**, 30, e202400784.
39. **Metallomimetic C-F activation catalysis by simple phosphines**, S. Bonfante, C. Lorber,\* J. M. Lynam,\* [A. Simonneau](#)\* and J. M. Slattery,\* *J. Am. Chem. Soc.* **2024**, 146, 2005-2014. **Most read article of January 2024, highlighted in C&EN.**
38. **An orbitally adapted semi-metallic frustrated Lewis pair template for N<sub>2</sub> activation and reduction to diazene-diide**, D. Specklin, M.-C. Boegli, A. Coffinet, L. Escomel, L. Vendier, M. Grellier and [A. Simonneau](#)\*, *Chem. Sci.* **2023**, 14, 14262–14270.
37. **Protonation Behavior of a Tetrahydrido Molybdenum(IV) Complex with Organic and Inorganic Acids**, N. Queyriaux,\* N. Durvin, D. Leon, M.-C. Boegli, L. Vendier and [A. Simonneau](#)\*, *Eur. J. Inorg. Chem.* **2023**, 26, e202300426.
36. **An Experimental and Computational Investigation Rules Out Direct Nucleophilic Addition on the N<sub>2</sub> Ligand in Manganese Dinitrogen Complex [Cp(CO)<sub>2</sub>Mn(N<sub>2</sub>)]**, Q. Le Dé, A. Bouammali, C. Bijani, L. Vendier, I. del Rosal, D. A. Valyaev,\* C. Dinoi\* and [A. Simonneau](#)\*, *Angew. Chem. Int. Ed.* **2023**, 62, e202305235 (**Very Important Paper**).
35. **CO<sub>2</sub> Hydroboration: Impact of the Boryl Moieties on the Reactivity of Four Bis(boryl)acetal Compounds toward 2,6-Diisopropylaniline**, S. Desmons, Y. Zhou, D. Zhang, C. Jarava-Barrera, A. Coffinet, [A. Simonneau](#), L. Vendier, G. Luo\* and S. Bontemps,\* *Eur. J. Org. Chem.* **2023**, 26, e202300525.
34. **Biomimetic catalysis of nitrite reductase enzyme using copper complexes in chemical and electrochemical reduction of nitrite**, M. P. Ferreira, C. B. Castro, J. Honorato, S. He, W. G. G. Júnior, C. Esmieu, E. E. Castellano, A. F. de Moura, D. R. Truzzi, O. R. Nascimento, [A. Simonneau](#) and C. G. C. M. Netto,\* *Dalton Trans.* **2023**, 52, 11254–11264.
33. **Assessing Combinations of Strong Lewis Acids and N<sub>2</sub>-derived Molybdenum Nitrido Complexes for Heterolytic Bond Activations**, A. Coffinet, Q. Le Dé, D. Specklin, S. Benaamane, L. Muñoz, L. Vendier, N. Mézailles\* and [A. Simonneau](#)\*, *Chem. Eur. J.* **2023**, 29, e202203774.
32. **Syntheses of N<sub>2</sub>-bridged heterobimetallic complexes, their structural and qualitative bonding analyses**, Q. Le Dé, F. Orbay, L. Vendier and [A. Simonneau](#)\*, *J. Organomet. Chem.* **2023**, 986, 122604.
31. **Dinitrogen-derived (diarylboryl)diazenido Complexes with Differing Coordination to the Thallium Cation**, A. Bouammali, A. Coffinet, L. Vendier and A. Simonneau,\* *Dalton Trans.* **2022**, 51, 10697–10701.
30. **Transition Metal-mediated Dinitrogen Functionalisation with Boron**, [A. Simonneau](#)\*, *New J. Chem.* **2021**, 45, 9294–9301.
29. **Borane-catalysed Dinitrogen Borylation by 1,3-B–H Bond Addition**, A. Coffinet, D. Zhang, L. Vendier, S. Bontemps and [A. Simonneau](#)\*, *Dalton Trans.* **2021**, 50, 5582–5589.
28. **Synthesis, Characterization, and Comparative Theoretical Investigation of Dinitrogen-Bridged Group 6-Gold Heterobimetallic Complexes**, D. Specklin, A. Coffinet, L. Vendier, I. del Rosal, C. Dinoi,\* [A. Simonneau](#)\*, *Inorg. Chem.* **2021**, 60, 5545–5562.
27. **Reaction of Methyllithium with Group 6 Phosphine Dinitrogen Complexes**, A. Bouammali, C. Bijani, L. Vendier, M. Etienne and [A. Simonneau](#)\*, *Eur. J. Inorg. Chem.* **2020**, 1423–1427.
26. **Frustrated Lewis Pair Chemistry Enables N<sub>2</sub> Borylation by Formal 1,3-Addition of a B–H Bond in the Coordination Sphere of Tungsten**, A. Coffinet, D. Specklin, L. Vendier, M. Etienne and [A. Simonneau](#)\*, *Chem. Eur. J.* **2019**, 25, 14300–14303.
25. **Enhanced Activation of Coordinated Dinitrogen with p-Block Lewis Acids (Concept)**, [A. Simonneau](#)\* and M. Etienne, *Chem. Eur. J.* **2018**, 24, 12458–12463 (**Reviews Showcase**).

24. **Group 6 Transition Metal/Boron Frustrated Lewis Pair Templates Activate N<sub>2</sub> and Allow its Facile Borylation and Silylation**, [A. Simonneau](#),\* R. Turrel, L. Vendier and M. Etienne, *Angew. Chem. Int. Ed.* **2017**, *56*, 12268-12272 (*Hot Paper*).

**Peer-reviewed journals – under mentorship**

23. **Review on Bioorganometallic Chemistry and New Outcomes in the Synthesis and Substitution of Tetracarbonyl(pyrrolylimine) Complexes of Rhenium with Organophosphorus Ligands**, [A. Simonneau](#),\* F. Le Bideau,\* J.-H. Mirebeau, J. Marrot and G. Jaouen, *Curr. Top. Med. Chem.* **2017**, *17*, 2807–2819.
22. **Assessing Ligand and Counterion Effects in the Noble Metal Catalyzed Cyclo-isomerization Reactions of 1,6-Allenynes: a Combined Experimental and Theoretical Approach**, F. Jaroschik, [A. Simonneau](#), G. Lemièrè, K. Cariou, N. Agenet, H. Amouri, C. Aubert, J.-P. Goddard, D. Lesage, M. Malacria, Y. Gimbert,\* V. Gandon\* and L. Fensterbank,\* *ACS Catal.* **2016**, *6*, 5146–5160.
21. **An Air-stable Dimeric Ruthenium NHC Complex as Catalyst for Hydrosilylation and Dehydrogenative Coupling Reactions**, S. Bähr, [A. Simonneau](#), E. Irran et M. Oestreich,\* *Organometallics* **2016**, *35*, 925–928.
20. **Formal SiH<sub>4</sub> Chemistry Using Stable and Easy-to-Handle Surrogates**, [A. Simonneau](#) and M. Oestreich,\* *Nat. Chem.* **2015**, *7*, 816–822. Highlighted in *Synfacts* and *Nachr. Chem.*
19. **The Cyclohexadienyl-Leaving-Group Approach Toward Donor-Stabilized Silylium Ions**, [A. Simonneau](#),\* T. Biberger and M. Oestreich,\* *Organometallics* **2015**, *34*, 3927–3929.
18. **Fascinating Hydrogen Atom Transfer Chemistry of Alkenes Inspired by Problems in Total Synthesis (Highlight)**, [A. Simonneau](#) and M. Oestreich,\* *Angew. Chem. Int. Ed.* **2015**, *54*, 3626–3628.
17. **Direct and Transfer Hydrosilylation Reactions Catalyzed by Fully or Partially Fluorinated Triarylboranes : A Systematic Study**, S. Keeß, [A. Simonneau](#) and M. Oestreich,\* *Organometallics* **2015**, *34*, 1237–1244.
16. **Salt-Free Preparation of Trimethylsilyl Ethers by B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>-Catalyzed Transfer Silylation Using a Me<sub>3</sub>SiH Surrogate**, [A. Simonneau](#), J. Friebel and M. Oestreich,\* *Eur. J. Org. Chem.* **2014**, 2077–2083. Highlighted in *Organic Chemistry Highlights*.
15. **Two-fold Tandem Acyl-Group Shift/Cyclization via Gold Catalysis**, [A. Simonneau](#), G. Maestri, L. Fensterbank\* and M. Malacria,\* *Arkivoc* **2014**, 287–296.
14. **3-Silylated Cyclohexa-1,4-dienes as Precursors for Gaseous Hydrosilanes: The B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>-Catalyzed Transfer Hydrosilylation of Alkenes**, [A. Simonneau](#) and M. Oestreich,\* *Angew. Chem. Int. Ed.*, **2013**, *52*, 11905–11907. Highlighted in *Synfacts*.
13. **Atroposelective [2+2+2] Cycloadditions Catalyzed by a Rhodium/Chiral Phosphate System**, M. Augé, M. Barbazanges-Aubry, A.-T. Tran, [A. Simonneau](#), P. Elley, H. Amouri, C. Aubert,\* L. Fensterbank,\* V. Gandon, M. Malacria and C. Ollivier,\* *Chem. Commun.*, **2013**, *49*, 7833–7835. Highlighted in *Synfacts*.
12. **Ring Expansions Within Gold-catalyzed Cycloisomerization of O-tethered 1,6-enynes. Application to the Synthesis of Natural Product-like Macrocycles**, [A. Simonneau](#), Y. Harrak, L. Jeanne-Julien, G. Lemièrè, V. Mouriès-Mansuy, J.-P. Goddard, M. Malacria and L. Fensterbank,\* *ChemCatChem*, **2013**, *5*, 1096–1099. **Back cover of the issue.**
11. **Tracking Gold Acetylides in Gold(I)-Catalyzed Cycloisomerization Reactions of Enynes**, [A. Simonneau](#), F. Jaroschik, D. Lesage, M. Karanik, R. Guillot, M. Malacria, J.-C. Tabet, J.-P. Goddard, L. Fensterbank,\* V. Gandon\* and Y. Gimbert,\* *Chem. Sci.*, **2011**, *2*, 2417–2422.
10. **Combination of Gold Catalysis and Selectfluor for the Synthesis of Fluorinated Nitrogen Heterocycles**, [A. Simonneau](#), P. Garcia, J.-P. Goddard, V. Mouriès-Mansuy, M. Malacria\* and L. Fensterbank,\* *Beilstein J. Org. Chem.*, **2011**, *7*, 1379–1386.
9. **Pentamethylcyclopentadienyl)Iridium Dichloride Dimer {[IrCp\*Cl<sub>2</sub>]<sub>2</sub>}: a Novel Efficient Catalyst for the Cycloisomerizations of Homopropargylic Diols and N-tethered Enynes**, E. Benedetti, [A. Simonneau](#), A. Hours, H. Amouri, A. Penoni, G. Palmisano, M. Malacria,\* J.-P. Goddard and L. Fensterbank,\* *Adv. Synth. Catal.*, **2011**, *353*, 1908–1912.
8. **Gold-catalyzed 1,3-Acyloxy Migration/5-exo-dig Cyclization/1,5-Acyl Migration of Diynyl Esters**, D. Leboeuf, [A. Simonneau](#), C. Aubert, M. Malacria,\* V. Gandon\* and L. Fensterbank,\* *Angew. Chem. Int. Ed.*, **2011**, *50*, 6868–6871.
7. **Transition Metal Catalyzed Cycloisomerizations of 1,n-Allenynes and -Allenenes**, C. Aubert,\* L. Fensterbank,\* P. Garcia, M. Malacria,\* and [A. Simonneau](#), *Chem. Rev.*, **2011**, *111*, 1954–1993.
6. **Gold(I)-Catalysed Cycloisomerisation of 1,6-Enynes into Functionalised Allenes**, Y. Harrak, [A. Simonneau](#), M. Malacria,\* V. Gandon\* and L. Fensterbank,\* *Chem. Commun.*, **2010**, *46*, 865–867.

**Book Chapters and Monographs**

5. **Push–Pull Activation of N<sub>2</sub> : Coordination of Lewis Acids to Dinitrogen Complexes**, A. Coffinet, A. Simonneau and D. Specklin, in *Encyclopedia of Inorganic and Bioinorganic Chemistry*, R.A. Scott (Ed.), John Wiley & Sons, Ltd, 2020, DOI: 10.1002/9781119951438.eibc2755.
4. **3-(Trimethylsilyl)-1,4-cyclohexadiene**, [A. Simonneau](#) and M. Oestreich, in *Electronic Encyclopedia of Reagents for Organic Synthesis*, D. Crich, P. L. Fuchs, A. B. Charette, T. Rovis (Eds.), Wiley: Chichester, Royaume-Uni, 2016, DOI: 10.1002/047084289X.m01910.
3. **Gold-Catalyzed Cycloisomerization Reactions Through Activation of Alkynes**, [A. Simonneau](#), Springer International Publishing Switzerland, 2014.

2. **Gold-Catalyzed Reactions of Propargylic Esters**, L. Fensterbank, J.-P. Goddard, M. Malacria and [A. Simonneau](#) in *Gold Catalysis: An Homogeneous Approach*, V. Michelet, F. D. Toste (Eds.), Imperial College Press : Londres, Royaume-Uni, 2014, pp 331–391.

#### Patents

1. **Use of Cyclohexa-2,5-dien-1-yl-silanes as Precursors for Gaseous Hydrosilanes**, [A. Simonneau](#) and M. Oestreich, *PCT Int. Appl.* WO 2015/036309 A1.

### COMMUNICATIONS AND LECTURES

27. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, invited lecture, *Journées de Chimie de Coordination*, Sacaly, France, **January 2025**.
26. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, invited lecture, *Institut de Chimie Moléculaire de Bourgogne*, Dijon, France, **November 2024**.
25. **A Pentahydro Molybdenum Complex for Small Molecule Activation and Hydrogenation Catalysis**, oral communication, *XLII Reunión del GEQO*, Sevilla, Spain, **September 2024**.
23. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, oral communication, *European Colloquium on Inorganic Reaction Mechanisms*, Toulouse, France, **September 2024**.
23. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, oral communication, *International Congress of Coordination Chemistry*, Fort Collins, USA, **July 2024**.
22. **Metallomimetic C–F Activation Catalysis by Simple Phosphines**, oral communication, *International Congress of Catalysis*, Lyon, France, **July 2024**.
21. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, invited lecture, *Institut Charles Gerhardt*, Montpellier, France, **May 2024**.
20. **Activation of the Carbon-Fluorine Bond: from Metal Mediation to Metal-Free Catalysis**, oral communication, *Journées de Printemps de la Division de Chimie Organique*, Paris, France, **April 2024**.
19. **Metallomimetic C–F Activation Catalysis by Simple Phosphines**, oral communication, *Journées de Chimie de Coordination*, Strasbourg, France, **January 2024**.
18. **Vintage Organometallic Chemistry — Tales of Surprises and Serendipity**, invited lecture, *URCOM*, Université du Havre, France, **January 2024**.
17. **Activation of Small Molecules and Strong Bonds with a Vintage Flavour**, invited lecture, *Chimie ParisTech*, Paris, France, **October 2023**.
16. **Mid Transition Metal Complexes for Small Molecule Activation**, invited lecture, *Département de Chimie Moléculaire, Université Grenoble Alpes*, Grenoble, France, **June 2023**.
15. **Nucleophilic Addition on Coordinated N<sub>2</sub>: Fact or Fiction?**, oral communication, *GECOM-CONCOORD*, Fournols, France, **May 2023**.
14. **Revisiting N<sub>2</sub> Functionalization with Nucleophiles**, oral communication, *Journées de Chimie Organique*, Palaiseau, France, **November 2022**.
13. **Revisiting N<sub>2</sub> Functionalization with Nucleophiles**, oral communication, *ICOMC*, Prague, Czech Republic, **July 2022**.
12. **Electrophiles vs. Nucleophiles: What's the Best to Transform Dinitrogen?**, invited lecture, *Institut de Chimie de Toulouse*, **July 2022**.
11. **Metal-Boron Cooperation for Dinitrogen and Hydrogen Activation**, invited lecture, *Faculty of Chemistry of the National Autonomous University of Mexico*, **June 2022**.
10. **Metal-Boron Cooperation: From Stoichiometric Activation of Small Molecules to Catalysis**, oral communication, *CEHC-2*, Leipzig, Germany, **March 2022**.
9. **Frustrated Lewis Pair Chemistry Inspires Nitrogen Fixation**, invited lecture, *PACIFICHEM*, Honolulu, United States of America (HI), **December 2020** (cancelled).
8. **Making Bonds between Dinitrogen and other Elements using Molecular Complexes**, keynote lecture, *GECOM-CONCOORD*, Camaret-sur-mer, France, **May 2020** (cancelled).
7. **Dinitrogen Activation with the Help of the Main Group**, invited lecture, *Department of Chemistry of the Federal University of São Carlos*, Brazil, **Feb. 2019**.
6. **Functionalization of Dinitrogen Induced by p-Block and Metal Lewis acids**, invited lecture, *Université Claude Bernard Lyon 1*, France, **Sept. 2018**.
5. **Dinitrogen Complexes and Lewis Acids: A Fruitful Collaboration**, oral communication, *International Conference on Coordination Chemistry*, Sendai, Japan, **Jul. 2018**.
4. **Group 6 Transition-Metal/Boron Frustrated Lewis Pair Templates for Dinitrogen Activation and its Functionalization**, oral communication, *Journées de Chimie de Coordination*, Brest, France, **Feb. 2018**.
3. **Transfer Hydrosilylation**, oral communication, *6<sup>th</sup> EuCheMS Chemistry Congress*, Seville, Spain, **Sep. 2016**.

2. **My Journey in Organometallic Catalysis: from Complex Cycloisomerization Reactions to Mechanisms, Ending up in Small Molecule Activation**, *LCC Welcome Lecture*, Toulouse, France, Dec. 2015.
1. **The Use of 3-Silylated Cyclohexa-1,4-dienes as Precursors for Gaseous Hydrosilanes**, oral communication, *17th International Symposium on Silicon Chemistry*, Berlin, Germany, Aug. 2014.

## COLLABORATIONS

### ■ Local level

S. Bontemps (LCC)	Boranes for small molecules functionalization, 2 publications.
C. Dinoi, I. del Rosal (LPCNO)	ERC-funded, DFT calculations, N <sub>2</sub> -complexes chemistry, 2 publications.
M. Grellier (LCC)	Région Occitanie-funded, hydrogen storage.
N. Mézailles (LHFA)	ERC-funded, chemistry of molecular Molybdenum nitrides with Lewis acids, 1 publication.
D. Valyaev (LCC)	ERC-funded, manganese-dinitrogen complexes, 1 publication.
N. Queyriaux (LCC)	ERC-funded, chemistry of molecular Molybdenum hydrides, 1 publication.
J.-B. Sortais (LCC)	Homogeneous hydrogenation catalysis with Molybdenum complexes.

### ■ National level

M. Gennari, C. Duboc (DCM, Univ. Grenoble-Alpes)	ANR-funded, homogeneous dinitrogen reduction.
K. Miqueu (IPREM, Univ. Pau)	DFT calculations, reactivity of Molybdenum hydrides.
R. Gauvin, L. Delevoye (IRCP, Chimie ParisTech, and UCCS, Univ. Lille)	Infranalytics-funded, high-field, solid-state NMR of molecular Molybdenum hydrides

### ■ International level

C. Gruenwaldt (Univ. São Carlos, Brazil)	Biomimetic copper and molybdenum complexes, 1 publication.
J. Lynam, J. Slattery (Univ. York, UK)	MSCA-funded, C–F bond activation, 1 publication.
N. Farfàn, R. Santillan (UNAM, Mexico)	CNRS-funded, dipyrromethene ligands for early transition metals.
V. Krewald (TU Darmstadt, Germany)	DFT calculations, N <sub>2</sub> -complexes chemistry, 1 publication.
M. Drover (Western University, Canada)	France-Canada Research Fund & French Ministry of Research and Higher Education Base metals / boron cooperative systems for small molecule activation

## NON-PROFESSIONAL OCCUPATIONS

since 2022 Secretary of the "loi 1901" association "L'Escapade Club" promoting the practice of outdoor sport climbing.