

Dr. Antoine Simonneau

ORCID iD: 0000-0003-4612-284X

Researcher iD: A-7296-2016

Laboratoire de Chimie de Coordination,
205 route de Narbonne, 31077 Toulouse cedex 4, France.

born March 6, 1985, French nationality

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

2 children (born 2015 and 2017)

email: antoine.simonneau@lcc-toulouse.fr

phone: +33 (0)5 61 33 31 44

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_2 , H_2 , CO_2) 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 **9th December 2011**, issued **11th 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

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

PhD supervision

2017–2020	Anaïs Coffinet (Univ. Toulouse), 100% supervision rate.
2018–2022	Amal Bouammali (Univ. Toulouse), 100% supervision rate.
2019–2023	Quentin Le Dé (Univ. Toulouse), 100% supervision rate.
2020–2024	Marie-Christine Boegli (Univ. Toulouse), 100% supervision rate.
2020–2024	Sara Bonfante (Univ. Toulouse and Univ. of York), co-supervision (50%) with Dr. John Slattery.
2021–2025	Arno Estival (Univ. Toulouse), co-supervision (50%) with Dr. Mary Grellier, LCC-University of Toulouse.
2024	Luis Blancarte (Autonomous National University of Mexico), research stay.
2024–	Quentin Lepeintre (Univ. Toulouse), co-supervision (50%) with Prof. M. Drover, Western University (Canada).

Postdoc supervision

2018–2021	Dr. David Specklin.
2020–2022	Dr. Nicolas Queyriaux
2023–2025	Dr. Léon Escomel.
2025–2026	Dr. Michel Sigrist.

Participation to PhD defense committees

Dec. 2020	Lydia Merakeb (LEM, Univ. Paris-Cité), examiner.
Nov. 2023	Vincent Wowk (i-CLeHS, Chimie ParisTech), reviewer.
Jan. 2024	Mathieu Pascaretti (URCOM, Univ. Le Havre), reviewer.
Sep. 2024	Francesco Crisanti (LEM, Sorbonne Univ.), examiner.
June 2025	Adrien Combourrieu (LCM, Institut Polytechnique de Paris), reviewer.
Jul. 2025	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).
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TEACHING ACTIVITIES

Jun. 2022	2 nd 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 th 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 st and 3 rd 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	>35 reviews for the following journals (among others, please refer to my ORCID profile)
	Angew. Chem Int. Ed.
	J. Am. Chem. Soc.
	Chem. Sci.
	Nat. Commun.
	JACS Au
	Chem. Commun.
	Chem. Eur. J.
	Chem. Asian J.
	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	Member of the Organizing Committee of the GECOM-CONCOORD colloquium — Logistics & Sponsors crew , 20–24 May 2024, Ax-les-Thermes, France.
2020	Member of the Organizing Committee of the online colloquium “Cutting-edge Homogeneous Catalysis” (CEHC-1) , 4–6 May 2021, Toulouse, France.
2019–2020	Member of the Organizing Committee of the European Colloquium on Inorganic Reaction Mechanisms (ECIRM) , 12–15 July 2020, Toulouse, France (cancelled).

PROFESSIONAL TRAINING

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

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

2026	French National Research Agency (ANR) collaborative research grant. Public funding for fundamental research. Project “PICATA”, <u>principal investigator</u> • 320 k€.
2025	EMERGENCE International , 3 k€ travel grant.
2025–2026	EMERGENCE @CNRS Chimie grant. Covered 18-month postdoc salary + 15 k€. <u>Principal Investigator</u> .
2024–2027	Doctoral fellowship of the France-Canada Research Fund - French Ministry of research and Higher Education. Covered the salary of a PhD student over 3 years. <u>Co-principal investigator</u> .
2024–2026	France-Canada Research Fund. CA\$ 15 000 covering mobility expenses.
2024	INFRANALYTICS Project. 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	International Research Project granted by the CNRS. 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	French National Research Agency (ANR) collaborative research grant. Public funding for fundamental research. Project “PUNCh”, coordinated by M. Gennari, DCM, University of Grenoble-Alpes • 154 k€.
2021–2024	Green Hydrogen grant. Public funding for research on hydrogen and its applications. Project “CataLOHC”. <u>Principal Investigator</u> • 76 k€.
2020–2024	International Training Network “CCIMC”. 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	ERC Starting Grant. Covered among others salaries for 3 Ph.D. and 2 postdocs, equipment, travel and consumables. <u>Principal Investigator</u> • 1.5 M€.
2017–2020	Doctoral fellowship of the French Ministry of research and Higher Education. Covered the salary of a PhD student over 3 years.
2015–2017	“Nouveaux Entrants” fellowship. Seed money provided by the Université Fédérale Toulouse Midi-Pyrénées to help settlement of young researchers. <u>Principal Investigator</u> • 14 k€.
2014–2015	Alexander von Humboldt Research Fellowship. Covered salary and research costs for 18 months.

2017	AAPG ANR JCJC, project "MIDIFUNK" — PI, not funded .
2019	International Emerging Action, PI with Prof. C. Gruenwaldt (Univ. Sao Carlos, Brazil), not funded .
2021	Appel à projet ADEME, co-PI with S. Bontemps (LCC, team SMAc), not funded .
2023	ERC Call "Proof-of-Concept", project HYDRa — PI, not funded (Seal of Excellence obtained).
2024	AAPG ANR PRC, project "MnN's" — PI, not funded .
2024	AAPG ANR PRC, project "MimPhos" — partner (PI: C. Lorber, LCC, team SMAc), not funded .
2024	ERC Call "Proof-of-Concept", project HYDRa — PI, not funded (Seal of Excellence obtained).
2024	MSCA Call "Postdoctoral Fellowships", project MoBHy, not funded (Seal of Excellence obtained).

SCIENTIFIC PRODUCTIONS

A = article, C = communication, R = review, P = patent

Peer-reviewed journals – Independent career

- R49. **Polytopic Main-group Lewis Acids for the Coordination and Activation of Small Molecules (Review)**, L. Escomel* and A. Simonneau,* *Coord. Chem. Rev.* **2025**, 544, 216948..
- C48. **Reductive Cleavage of Dioxygen Mediated by a Lewis Superacidic Bis(Borane)**, L. Escomel, L. Vendier, D. Gatineau, F. Molton, C. Duboc, M. Gennari* and A. Simonneau,* *JACS Au* **2025**, DOI: 10.1021/jacsau.5c00516.
- A47. **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,* *Chem. Sci.* **2025**, 16, 3552–3559.
- A46. **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,* *Dalton Trans.* **2025**, 54, 2860–2870.
- A45. **Bio-Inspired Thiolate-Fell-Hydrazine Adduct Towards Iron-Mediated C-N Bond Formation**, I. Cassandrini, C. Philouze, A. Simonneau, C. Duboc and M. Gennari,* *Eur. J. Inorg. Chem.* **2025**, e202400633.
- A44. **Reactivity of Metal Hydrides with CO₂: 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**, 15, 20582–20589.
- C43. **Low-valent Group 6 Metals/Al(C₆F₅)₃ Donor-Acceptor Systems for CO₂ Activation and Cleavage**, L. Escomel, Q. Le Dé, M. Benonie, L. Vendier and A. Simonneau,* *Chem. Commun.*, **2024**, 60, 13235–13238.
- A42. **Coordination of Al(C₆F₅)₃ vs B(C₆F₅)₃ 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.
- A41. **Seven-coordinate Group 6 Metal Hydrides Obtained by H₂ Activation at B(C₆F₅)₃ Adducts of N₂ 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.
- R40. **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.
- A39. **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.**
- A38. **An orbitally adapted semi-metallic frustrated Lewis pair template for N₂ 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.
- A37. **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.
- A36. **An Experimental and Computational Investigation Rules Out Direct Nucleophilic Addition on the N₂ Ligand in Manganese Dinitrogen Complex [Cp(CO)₂Mn(N₂)], 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**).**
- A35. **CO₂ 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.
- A34. **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.
- A33. **Assessing Combinations of Strong Lewis Acids and N₂-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.
- A32. **Syntheses of N₂-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.
- A31. **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.

- R30. Transition Metal-mediated Dinitrogen Functionalisation with Boron, A. Simonneau,* *New J. Chem.* **2021**, 45, 9294–9301.
- A29. 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.
- A28. 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* and A. Simonneau,* *Inorg. Chem.* **2021**, 60, 5545–5562.
- A27. 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.
- A26. Frustrated Lewis Pair Chemistry Enables N₂ 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.
- R25. 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).
- C24. Group 6 Transition Metal/Boron Frustrated Lewis Pair Templates Activate N₂ 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

- R23. 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.
- A22. 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. Lemi re, 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.
- C21. An Air-stable Dimeric Ruthenium NHC Complex as Catalyst for Hydrosilylation and Dehydrogenative Coupling Reactions, S. B hr, A. Simonneau, E. Irran et M. Oestreich,* *Organometallics* **2016**, 35, 925–928.
- A20. Formal SiH₄ 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.*
- C19. The Cyclohexadienyl-Leaving-Group Approach Toward Donor-Stabilized Silylium Ions, A. Simonneau,* T. Biberger and M. Oestreich,* *Organometallics* **2015**, 34, 3927–3929.
- R18. 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.
- A17. Direct and Transfer Hydrosilylation Reactions Catalyzed by Fully or Partially Fluorinated Triarylboranes : A Systematic Study, S. Kee , A. Simonneau and M. Oestreich,* *Organometallics* **2015**, 34, 1237–1244.
- A16. Salt-Free Preparation of Trimethylsilyl Ethers by B(C₆F₅)₃-Catalyzed Transfer Silylation Using a Me₃SiH Surrogate, A. Simonneau, J. Friebe and M. Oestreich,* *Eur. J. Org. Chem.* **2014**, 2077–2083. Highlighted in *Organic Chemistry Highlights*.
- C15. Two-fold Tandem Acyl-Group Shift/Cyclization via Gold Catalysis, A. Simonneau, G. Maestri, L. Fensterbank* and M. Malacria,* *Arkivoc* **2014**, 287–296.
- C14. 3-Silylated Cyclohexa-1,4-dienes as Precursors for Gaseous Hydrosilanes: The B(C₆F₅)₃-Catalyzed Transfer Hydrosilylation of Alkenes, A. Simonneau and M. Oestreich,* *Angew. Chem. Int. Ed.*, **2013**, 52, 11905–11907. Highlighted in *Synfacts*.
- C13. Atroposelective [2+2+2] Cycloadditions Catalyzed by a Rhodium/Chiral Phosphate System, M. Aug , 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*.
- C12. 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. Lemi re, V. Mouri s-Mansuy, J.-P. Goddard, M. Malacria and L. Fensterbank,* *ChemCatChem*, **2013**, 5, 1096–1099. Back cover of the issue.
- A11. 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.
- A10. Combination of Gold Catalysis and Selectfluor for the Synthesis of Fluorinated Nitrogen Heterocycles, A. Simonneau, P. Garcia, J.-P. Goddard, V. Mouri s-Mansuy, M. Malacria* and L. Fensterbank,* *Beilstein J. Org. Chem.*, **2011**, 7, 1379–1386.
- C9. Pentamethylcyclopentadienyl)Iridium Dichloride Dimer {IrCp*Cl₂]₂: 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.
- C8. 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.
- R7. 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.

- C6. **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

- R5. **Push–Pull Activation of N₂: 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.
- R4. **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.
- R2. **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

- P1. **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

IL = invited lecture, IC = invited contribution in a conference, OC = oral communication

- IC33. **Interplay of electron-rich metal species and Lewis acids for the activation of small molecules**, *Main-group Elements Reactivity Conference*, Namur, Belgique, **September 2025**.
- OC32. **Implementing Lewis SuperAcids (LSA) in Hybrid Main Group/Metal Donor-Acceptor Systems for Small Molecules Activation**, *European Conference on Organometallic Chemistry*, Bern, Switzerland, **July 2025**.
- IL27-31. **Interplay of Electron-rich Metal Species and Lewis Acids for the Activation of Small Molecules**, lecture tour in the United Kingdom in the frame of the Emergence International funding scheme provided by CNRS Chimie. Talks delivered at the *University of York*, the *University of Cambridge*, the *Imperial College*, the *University of Bath* and the *University of Cardiff*, **May 2025**.
- IC26. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, *Journées de Chimie de Coordination*, Saclay, France, **January 2025**.
- IL25. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, *Institut de Chimie Moléculaire de Bourgogne*, Dijon, France, **November 2024**.
- OC24. **A Pentahydrido Molybdenum Complex for Small Molecule Activation and Hydrogenation Catalysis**, *XLII Reunión del GEQO*, Sevilla, Spain, **September 2024**.
- OC23. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, *European Colloquium on Inorganic Reaction Mechanisms*, Toulouse, France, **September 2024**.
- OC22. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, *International Congress of Coordination Chemistry*, Fort Collins, USA, **July 2024**.
- OC21. **Metallomimetic C–F Activation Catalysis by Simple Phosphines**, *International Congress of Catalysis*, Lyon, France, **July 2024**. Best presentation award.
- IL20. **Molecular Donor-Acceptor Systems for Small Molecules Activation**, *Institut Charles Gerhardt*, Montpellier, France, **May 2024**.
- OC19. **Activation of the Carbon-Fluorine Bond: from Metal Mediation to Metal-Free Catalysis**, *Journées de Printemps de la Division de Chimie Organique*, Paris, France, **April 2024**.
- OC18. **Metallomimetic C–F Activation Catalysis by Simple Phosphines**, *Journées de Chimie de Coordination*, Strasbourg, France, **January 2024**.
- IL17. **Vintage Organometallic Chemistry — Tales of Surprises and Serendipity**, *URCOM*, Université du Havre, France, **January 2024**.
- IL16. **Activation of Small Molecules and Strong Bonds with a Vintage Flavour**, *Chimie ParisTech*, Paris, France, **October 2023**.
- IL15. **Mid Transition Metal Complexes for Small Molecule Activation**, *Département de Chimie Moléculaire, Université Grenoble Alpes*, Grenoble, France, **June 2023**.
- OC14. **Nucleophilic Addition on Coordinated N₂: Fact or Fiction?**, *GECOM-CONCOORD*, Fournols, France, **May 2023**.
- OC13. **Revisiting N₂ Functionalization with Nucleophiles**, *Journées de Chimie Organique*, Palaiseau, France, **November 2022**.
- OC12. **Revisiting N₂ Functionalization with Nucleophiles**, *ICOMC*, Prague, Czech Republic, **July 2022**.
- IL11. **Electrophiles vs. Nucleophiles: What's the Best to Transform Dinitrogen?**, *Institut de Chimie de Toulouse*, **July 2022**.
- IL10. **Metal-Boron Cooperation for Dinitrogen and Hydrogen Activation**, *Faculty of Chemistry of the National Autonomous University of Mexico*, **June 2022**.

- OC9. **Metal-Boron Cooperation: From Stoichiometric Activation of Small Molecules to Catalysis**, *CEHC-2*, Leipzig, Germany, March 2022.
- IC8. **Frustrated Lewis Pair Chemistry Inspires Nitrogen Fixation**, *PACIFICHEM*, Honolulu, United States of America (HI), December 2020 (cancelled).
- IC7. **Making Bonds between Dinitrogen and other Elements using Molecular Complexes**, *GECOM-CONCOORD*, Camaret-sur-mer, France, May 2020 (cancelled).
- IL6. **Dinitrogen Activation with the Help of the Main Group**, *Department of Chemistry of the Federal University of São Carlos*, Brazil, Feb. 2019.
- IL5. **Functionalization of Dinitrogen Induced by p-Block and Metal Lewis acids**, *Université Claude Bernard Lyon 1*, France, Sept. 2018.
- OC4. **Dinitrogen Complexes and Lewis Acids: A Fruitful Collaboration**, *International Conference on Coordination Chemistry*, Sendai, Japan, Jul. 2018.
- OC3. **Group 6 Transition-Metal/Boron Frustrated Lewis Pair Templates for Dinitrogen Activation and its Functionalization**, *Journées de Chimie de Coordination*, Brest, France, Feb. 2018.
- OC2. **Transfer Hydrosilylation**, 6th EuCheMS Chemistry Congress, Seville, Spain, Sep. 2016.
- IL1. **My Journey in Organometallic Catalysis: from Complex Cycloisomerization Reactions to Mechanisms, Ending up in Small Molecule Activation**, *LCC Welcome Lecture*, Toulouse, France, Dec. 2015.

COLLABORATIONS

■ Local level

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

■ National level

M. Gennari, C. Duboc (DCM, Univ. Grenoble-Alpes)	ANR-funded, homogeneous dinitrogen reduction, 2 publications.
K. Miqueu (IPREM, Univ. Pau)	DFT calculations, reactivity of Molybdenum hydrides, 1 publication.
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, 2 publications.
N. Farfàn, R. Santillan (UNAM, Mexico)	CNRS-funded, dipyrromethene ligands for early transition metals, 1 publication.
V. Krewald (TU Darmstadt, Germany)	DFT calculations, N ₂ -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 sport climbing through courses and outdoor practice.
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