Dr Pierre-Adrien PAYARD
French, 31 years old
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UE driving license

Mechanisms: Prediction Tools for Reaction Development

My research is dedicated to understanding and modeling of complex catalytic systems on a molecular level through a multidisciplinary approach: at the interface between advanced physicochemical characterization and multi-scale computer modeling. I started my independent career as associate professor at the University of Lyon in 2020 and am currently co-directing a team of five PhD students, one postdoc and several master students. I am passionate about comprehending and overcoming catalytic limitations encountered by synthetic chemists, thus we are involved in numerous collaborations at the national and international level, with academic and industrial partners.

Current Position

2020-current **Associate Professor at Université Claude Bernard Lyon 1**
Institut de Chimie et de Biochimie Moléculaires et Supramoléculaires (ICBMS)
www.icbms.fr/fr/equipe/3-itemm-html

Education

2016-2019 **PhD in Physical Organic Chemistry at Ecole Normale Supérieure**
Under the supervision of Dr L. Grimaud and Prof M. Pera-Titus
Mechanistic Studies of Metal-Catalyzed Reactions: Predicting Tools for Reaction Optimization.
Ecole Normale Supérieure / Université PSL, France / UMI E2P2, Solvay-CNRS, China.
laurence.grimaud@ens.fr peratitusm@cardiff.ac.uk raphael.wischert@solvay.com

2016 **"Agrégation de Physique-Chimie" / Master's Degree in Teaching Science**
Major: Chemistry - Minor: Physics
ENS Paris-Saclay, France

2015 **Master's Degree in Molecular Chemistry** *with highest honors*
Sorbonne Université, France.

Master's Degree in Physical and Molecular Chemistry *with highest honors*
ENS Paris-Saclay / Université Paris Saclay, France.

Work experience

2019-2020 **Postdoctoral Researcher at ETH Zurich,**
Advisor Prof. Dr. C. Copéret
Rational Design of Well-Defined Polymetallic Catalysts for Fuel and Energy.
ETH Zurich, Inorganic Chemistry Laboratory, Zurich, Switzerland
ccoperet@inorg.chem.ethz.ch

2015 **Research Project Ni-Catalyzed Suzuki Coupling: Mechanistic Study (5 months)**
Supervised by Dr L. Grimaud.
Laboratoire PASTEUR, UMR ENS-CNRS-UPMC, Paris, France

2014 **Research Project, Lewis-Superacid-Catalyzed Amination of Alcohol (6 months)**
Supervised by Dr M. Corbet and Dr D. Cartigny
E2P2 lab, UMI Solvay-CNRS, Shanghai, China

Professional skills

Languages French (native speaker), English (fluent, C1), German (Intermediate, B1), Chinese (basic knowledge), Spanish (basic knowledge)

Computational Skills Office, LaTeX, *Chemical structure drawing:* ChemDraw, *Data treatment:* Origin, Gnuplot, *Quantum Chemistry:* Gaussian, Turbomol, ORCA, VASP, CP2K, USPEX, Hyperchem, Spartan, Gaussview, Material Studio, *Database:* EndNote, *programming knowledge: python, bash, perl, c.*

Experimental Skills *Electrochemistry*, Kinetic, Mechanisms, Catalysis, Organic and Organometallic Synthesis, NMR (^{1}H, ^{13}C, ^{19}F, ^{31}P, ^{11}B), GC/HPLC, EPR, FTIR, Surface Chemistry (SOMC), *XAS*, Gas-phase catalytic tests (batch and flow), *DFT (molecular and periodic), Ab initio Molecular Dynamics, Machine Learning.*

Academic Achievements (see also Publications List)

Supervision of Students
2022-2023 5 PhD students, 1 postdoc.
2021-2022 3 PhD students, 5 Master students.
2019-2020 1 PhD student, 3 Master students.
2016-2019 3 Master students, 5 undergraduate students.

Congress Planning French-Chinese conference on Green Chemistry (FC2GChem)

Academic Partners Dr. L. Perrin, Dr J. Vantourout, Prof. F. Popowyck (ICBMS, Univ. Lyon 1), Dr. R. Jazzar (Univ. California), Dr. J.-L. Hazemann (ESRF), Prof. C. Copéret (ETH Zurich), Prof. O. Eisenstein (Univ. Montpellier), Dr. O. Safonova (PSI Villigen), Prof. E. Hevia (Univ. Bern), Dr. I. Ciofini (ENSCP, PSL), Prof. B. Weckhuysen (Univ. Utrecht), Prof. M. Cascella (Univ. Oslo).

Industrial Partners Shell (Dr. S. van Bavel), IFPEN (Dr. R. Huyghe), Michelin (joint lab "ChemistLab"), IBM (Dr. A. Thukkar) Solvay (Dr. R. Wischert), Janssen (Dr. S. Magschal, Dr. L. Perego).

Prices & distinctions Nominated "young organic researcher to watch" (#NextGenOrgChem); Oral Communication Award (16ème RCO, jury: Prof. C. Bolm and Prof. C. Mazet); PhD Fellowship ENS; Ranked 13th out of 710 at the Agrégation of Chemistry.

Reviewing activities Early Career Editorial Board of the Journal of Catalysis. Reviewer for JACS, JACS Au, ACS Catal., Theor. Chem. Acc., Top. Catal.

Research Fundings

2023-2024 GENCI, 6 million of CPU h.
2023 ESRF, FAME-UHD, 18 shifts.
2023-2027 Michelin, postdoc fellowship and 50 k€
2022-2026 Minister for research, PhD Fellowship.
2022 SLS / PSI, SuperXAS, 9 shifts.
2022-2026 ANR-SNF, Pt-NMR, 70 k€.
2022-2026 Chinese Research Council, PhD Fellowship.
2022-2023 GENCI, 4.5 million of CPU h.
2021-2025 ANR-Michelin, postdoc and 40 k€.
2021-2022 Univ Lyon 1, 10 k€.
2021-2023 Minister for research, PhD Fellowship.
2021-2022 GENCI, 5.6 million of CPU h.
2021-2023 Région ARA, ERC prep. fund, 20 k€
2020-2024 Chinese Research Council, PhD Fellowship
2020-2021 Univ Lyon 1, 10 k€

Teaching Activities

Since 2020 Lecturer at University of Lyon (Univ Lyon 1 and ENS Lyon)
Since 2021 Member of the jury of the entrance examination to ENS
2019 Member of the Scientific Committee of the IChO 2019
2020-2016 Tutor at Ecole Normale Supérieure

Hobbies

Music: piano, chamber music (piano trio); **Reading; Sports:** hiking, biking, tennis.

Scientific Publications

Articles with equal contribution are indicated with P.-A. Payard‡
Articles with corresponding co-authorship are indicated with P.-A. Payard*

29. Shedding Light on the Hidden Roles of Lithium in the Nickel-Catalyzed Cross-Coupling of Aryl Ethers H. Liang, A. Borys, E. Hevia, M.-E. L. Perrin, P.-A. Payard,* *J. Am. Chem. Soc.* 10.1021/jacs.3c06647

28. Regime Switch in the Dual-Catalyzed Coupling of Alkyl Silicates with Aryl Bromides K. Jaouadi, M. Abdellaoui, E. Levernier, P.-A. Payard, E. Derat, T. Le Saux, C. Ollivier, S. Torelli, L. Jullien, R. Plasson, L. Fensterbank, L. Grimaud, *Chem. Eur. J.* **2023**, e202301780. 10.1002/chem.202301780

27. PdGa Alloying-Dealloying Processes under Reducing and CO_2 Hydrogenation Reaction Conditions from Metadynamics Simulations J. F. Baumgärtner, A. Müller, S. R. Docherty, A. Comas-Vives, P.-A. Payard,* C. Copéret, *under review.* 10.26434/chemrxiv-2023-qk5f7

26. Elucidating the Role of Lithium as Dopant in Li/MgO for Methane Coupling with Isotope Labelling and Solid State ^{13}C NMR. S.B.X.Y. Zhang, Z. Berkson, L. Lätsch, Q. Pessemesse, A. P. van Bavel, A. D. Horton, P.-A. Payard, C. Copéret, *Angew. Chem.* **2023**, e202307814 10.1002/anie.202307814

25. We Already Know Everything about Oxidative Addition to Pd(0) - Do We? J. Rio, H. Liang, Marie-Eve L. Perrin, L. A. Perego, L. Grimaud, P.-A. Payard,* *ACS Catal.* **2023**, *13*, 11399–11421. 10.1021/acscatal.3c01943

24. Ti-Doping in Silica-Supported PtZn Propane Dehydrogenation Catalysts: From Improved Stability to the Nature of the Pt-Ti Interaction. L. Rochlitz, J. W. A. Fischer, Q. Pessemesse, A. H. Clark, A. Ashuiev, D. Klose, P.-A. Payard, G. Jeschke, C. Copéret, *JACS Au*, **2023**, *3,* 1939–1951. doi: 10.1021/jacsau.3c00197

23. Ir-Na Cooperativity Controls the Diastereoselectivity of Borrowing Hydrogen C-C Alkylation on Isosorbide: Synthesis Methodology and Mechanistic Investigation. J. François, J. Rio, E. Jeanneau, M.-E. L. Perrin, M. Jacolot, P.-A. Payard,* F. Popowycza, *Org. Chem. Front.*, **2023**, *Advance Article*. doi: 10.1039/D3QO00700F

22. Assigning ^{1}H Chemical Shifts in Paramagnetic Mono and Bimetallic Surface Sites using DFT: a Case Study on the Union Carbide Polymerization Catalyst, A. Nobile, D. Trummer, Z. Berkson, M. Wörle, C. Coperet, P.-A. Payard,* *Chem. Sci.* **2023,** *14*, 2361-2368. doi: 10.1039/D2SC06827C

21. Role and Dynamics of Transition Metal Carbides in Methane Coupling, S. B. X. Y. Zhang, Q. Pessemesse, L. Lätsch, K. M. Engel, W. J Stark, A. P van Bavel, A. D Horton, P.-A. Payard,* C. Copéret, *Chem. Sci.* **2023**, doi: 10.1039/D3SC01054F

20. Copper-Catalyzed Homocoupling of Boronic Acids: A focus on B-to-Cu and Cu-to-Cu Transmetalations, A. Salamé, J. Rio, I. Ciofini, L. Perrin, L. Grimaud, P.-A. Payard, *Molecules,* 2022, *27*, 7517 doi: 10.3390/molecules27217517

19. Structure – Reactivity Relationship of Organo-zinc and -zincate Reagents: Key Elements towards Molecular Understanding J. Rio, L. Perrin, P.-A. Payard,* *Eur. J. Org. Chem.* **2022**, e202200906, doi: 10.1002/ejoc.202200906 (and cover 10.1002/ejoc.202201306).

18. Grafting of Group-10 Organometallic Complexes on Silicas: Differences and Similarities,

Surprises and Rationale D. Gioffrè, L. Rochlitz, P.-A. Payard, A. Yakimov, C. Copéret, *Helv. Chim. Acta* **2022**, *105*, e202200073. doi: 10.1002/hlca.202200073

17. A Robust and Efficient Propane Dehydrogenation Catalyst from Unexpectedly Segregated Pt_2Mn Nanoparticles L. Rochlitz, Q. Pessemesse, J. W. A. Fischer, D. Klose, A. H Clark, M. Plodinec, G. Jeschke, P.-A. Payard,* C. Copéret *J. Am. Chem. Soc.*, **2022**, *144*, 29, 13384–13393. doi: 10.1021/jacs.2c05618

16. Union Carbide Ethylene Polymerization Catalyst: From Uncovering Active Site Structures to Designing Molecularly-Defined Analogs Trummer, D.;‡ Nobile, A.;‡ Payard, P.-A.;‡ Ashuiev, A.; Kakiuchi, Y.; Klose, D.; Jeschke, G.; Copéret, C. *Chem. Sci.*, **2022**, *13*, 11091-11098. doi: 10.1039/D2SC04235E

15. Salt-Enhanced Oxidative Addition of Iodobenzene to Pd: an Inter-play Between Cation, Anion and Pd-Pd Cooperative Effects H. Liang, J. Rio, L. Perrin, P.-A. Payard,* *Inorg. Chem.*, **2022**, *61*, 20, 7935–7944. doi: 10.1021/acs.inorgchem.2c00565

14. Dynamics and Site Isolation: Keys to High Propane Dehydrogenation Performance of Silica-Supported PtGa Nanoparticles, P.-A. Payard, L. Rochlitz, K. Searles, L. Foppa, B. Leuthold, O. V. Safonova, A. Comas-Vives, C. Copéret, *J. Am. Chem. Soc. Au* **2021**, *1*, 9, 1445–1458. doi: 10.1021/jacsau.1c00212 (top 5 of the most read papers from JACS Au in July 2021)

13. Amides Synthesis by Copper-Catalyzed Oxidative Transformation of Nitriles in Presence of Iodonium Triflates, R. Sallio, C. Bermejo, P.-A. Payard, I. Fabre, P. Pakulski, I. Diachenko, S. Berteina-Raboin, I. Ciofini, L. Grimaud, I. Gillaizeau, *RSC Adv.*, **2021**, *11*, 15885-15889. doi: 10.1039/D1RA02305E

12. Role of Hemilabile Diphosphine Monoxides in Transmetalation: The Hidden Ligand of the Suzuki-Miyaura Coupling, P.-A. Payard,* A. Bohn, D. Tocqueville, S. Ajig, A. Dethoor, S. Wagscha, I. Ciofini, L. Grimaud, *Organometallics* **2021**, *40*, 1120–1128. doi: 10.1021/acs.organomet.1c00090

11. Metal-Free Visible-Light Synthesis of Arysulfonyl Fluorides: Scope and Mechanism, D. Louvel, A. Chelagha, J. Rouillon, P.-A. Payard, L. Khrouz, C. Monnereau, A. Tlili, *Chem. Eur. J.* **2021**, *27*, 8704-8708, doi: 10.1002/chem.202101056

10. Heterogeneous Alkane Dehydrogenation Catalysts Investigated *via* a Surface Organometallic Chemistry Approach, S. R. Docherty, L. Rochlitz, P.-A. Payard, C. Copéret, *Chem. Soc. Rev.* **2021**, *50*, 5806-5822, 10.1039/D0CS01424A

9. A DFT Protocol for the Prediction of ^{31}P NMR Chemical Shifts of Phosphine Ligands in First-Row Transition-Metal Complexes, P.-A. Payard,* L.A. Perego, L. Grimaud, I. Ciofini, *Organometallics* **2020**, *39*, 3121–3130. doi: 10.1021/acs.organomet.0c00309

8. Rational Optimization of Lewis-Acid Catalysts for Direct Alcohol Amination, Part 2 – Titanium Triflimide as New Active Catalyst, P.-A. Payard,* C. Finidori, L. Guichard, D. Cartigny, M. Corbet, L. Khrouz, L. Bonneviot, R. Wischert, L. Grimaud, M. Pera-Titus, *Eur. J. Org. Chem.* **2020,** 3225-3228. doi: 10.1002/ejoc.202000413

7. Rational Optimization of Lewis-Acid Catalysts for the Direct Amination of Alcohols, Part 1 – Activity Descriptors for Metal Triflates and Triflimides, P.-A. Payard,* C. Finidori, L. Guichard, D. Cartigny, M. Corbet, L. Khrouz, L. Bonneviot, R. Wischert, L. Grimaud, M. Pera-Titus, *Eur. J. Org. Chem.* **2020,** 3219-3224. doi: 10.1002/ejoc.202000229

6. Triflate Iron Salts as Precursor of Highly Active and Selective Catalyst for Solvent-Free Oxidation of Cyclohexane into KA Oil P. A. Payard L. Khrouz, L. Bonneviot, L. Grimaud, R. Wischert,

M. Pera-Titus, *Eur. J. Org. Chem.* **2020**, 3552-3559. doi : 10.1002/ejoc.202000263 (cover feature, *Eur. J. Org. Chem.*, **2020**, 3516, doi: 10.1002/ejoc.202000800).

5. Copper Reactivity can be Tuned to Catalyse the Stereoselective Synthesis of 2-deoxy Glycosides from Glycals, C. Palo-Nieto, A. Sau, R. Jeanneret, P.-A. Payard, M. B. Martins-Teixeira, I. Carvalho, L. Grimaud, M. C. Galan, *Org. Lett.* **2020**, *22*, 1991–1996. doi: 10.1021/acs.orglett.9b04525

4. Evidence for a Cooperative Mechanism Involving two Palladium(0) Centers in the Oxidative Addition of Iodoarenes, L.A. Perego, P.A. Payard, B. Haddou, I. Ciofini et L. Grimaud, *Chem Eur. J.*, **2018**, *24* (9), 2192-2199. doi: 10.1002/chem.201704899

3. Taming Nickel-Catalyzed Suzuki-Miyaura Coupling: A Mechanistic Focus on Boron-to-Nickel Transmetalation. P.-A. Payard, L.A. Perego, I. Ciofini, L. Grimaud., *ACS Catal.*, **2018**, *8* (6), 4812–4823. doi : 10.1021/acscatal.8b00933

2. Direct Amination of Alcohols Catalyzed by Aluminum Triflate: an Experimental and Computational Study, P.-A. Payard, Q. Gu, W. Guo, Q. Wang, J. Lai, M. Corbet, C. Michel, P. Sautet, L. Grimaud, R. Wischert and M. Pera-Titus, *Chem Eur J.*, **2018**, *24*, 14146- 14153. doi: 10.1002/chem.201801492

1. The drying of linseed oil investigated by Fourier transform infrared spectroscopy: Historical recipes and influence of lead compounds, L. de Viguerie, P.A. Payard, E. Portero, Ph. Walter, M. Cotte, *Prog. Org. Coat.*, **2016**, *93*, 46–60. doi: 10.1016/j.porgcoat.2015.12.010

Oral communications

8. Metadynamics Exploration of Supported Nanoparticles, Q. Pessemesse, J. Baumgartner, A. Müller, L. Rochlitz, A. Comas-Vives, C. Copéret, P.-A. Payard – *ICTAC – June 2022 – Lyon, France.*

7. Assigning Paramagnetic Proton Chemical Shifts in the Union Carbide Ethylene Polymerization Catalyst
A. G. Nobile, D. Trummer, Z. J. Berkson, C. Copéret. P.-A. Payard – *GECOM-CONCOORD – May 2022 – Sévrier, France.*

6. The Dynamic Structure of Supported Nanoparticles: Key to Alkanes Valorization P.-A. Payard, L. Rochlitz, Q. Pessemesse, O. V. Safonova, A. Comas-Vives, C. Copéret – *FC2HChem (Invited lecturer) – October 2021 – Lyon, France.*

5. Taming Boron-to-Transition-Metal Transmetalation: Insights from Mechanistic Studies. P.-A. Payard – *Invited lecturer – April 2021 – University of Montpelier, France.*

4. Taming Boron-to-Transition-Metal Transmetalation: Insights from Mechanistic Studies, P.A. Payard, L. A. Perego, A. Salamé, I. Ciofini and L. Grimaud - *GECOM-CONCOORD – May 2019 – Erquy, France.*

3. Iron Triflate Salts as Precursors of Highly Active and Selective Catalyst for the Solvent-Free Oxidation of Cyclohexane, P.-A. Payard, Y.-T. Zheng, W.-J. Zhou, L. Khrouz, L. Bonneviot, C. Michel, R. Wischert, L. Grimaud, M. Pera-Titus – ISGC (*International Symposium for Green Chemistry) – May 2019 – La Rochelle, France.*

2. Evidence for a Cooperative Mechanism Involving two Palladium(0) Centers in the Oxidative Addition of Iodoarenes, P. A. Payard, L. A. Perego, B. Haddou, I. Ciofini, L. Grimaud – *Journée de la Montagne Sainte Geneviève – June 2018 – Paris, France.*

1. Taming Nickel-Catalyzed Suzuki Coupling: A Mechanistic Study, P.A. Payard, L. A. Perego, I. Ciofini and L. Grimaud – *RCO (16 ème Rencontre de Chimie Organique) – April 2018 – Paris, France* - **oral communication award.**