



Curriculum Vitae

Philippe Sautet

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Professional address

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1- Education

- "Diplome d'Ingénieur de l'École Polytechnique de Paris", June 1985
- "Diplome d'Etudes Approfondies" in Inorganic Chemistry, Paris-Orsay University, June 1986
- Doctorate in Physical Chemistry, January 1989, Paris-Orsay University
- Habilitation to direct research, November 1994, Lyon 1 University

2- Positions

- Professor at the Chemical and Biomolecular Engineering department of UCLA, since June 30 2016
- Exceptional class director of research at CNRS, Ecole Normale Supérieure de Lyon, France, since 2011
- Director of the "Institut de Chimie de Lyon" 2007-2015 (1000 persons)
- First class director of research at CNRS, Ecole Normale Supérieure de Lyon, France, since 2005-2011
- Director of the « Laboratoire de Chimie », UMR CNRS, Ecole Normale Supérieure de Lyon, France, 2003- 2010 (90 persons)
- Director of research at CNRS, Institut de Recherche sur la Catalyse, Villeurbanne and Ecole Normale Supérieure de Lyon, France, 1995-2005
- Professor at the Ecole Polytechnique, Paris, 1993-2005
- Visiting Scientist, Lawrence Berkeley Laboratory (Berkeley, California), 1991-1992
- Chargé of research at CNRS, Institut de Recherche sur la Catalyse, Villeurbanne and Ecole Normale Supérieure de Lyon, France, 1988-1995

3- Awards

- Chevalier de l'ordre des palmes académiques (2015)
- Pierre Süe Grand Prize of the French Chemical Society (2012)
- Member of the French Academy of Sciences (elected in 2010)
- Chevalier de l'Ordre National du Mérite (2011)
- Paul Pascal Award of the French Academy of Science, 2008
- Silver Medal of the CNRS 2007
- Descartes-Huygens prize 1998, awarded by the Royal Netherlands Academy of Arts and Sciences

- Award of the Catalysis Division of the French Chemical Society 1993
- Bronze medal of the CNRS 1991
- Raymond Berr student research award of the École Polytechnique 1985

4- Research activities

- Computational Catalysis
- Theory of the electronic structure at the solid-gas interface
- Modeling of elementary steps of heterogeneous catalysis
- Calculation of the Scanning Tunnelling Microscopy images of surfaces; interpretation of images of adsorbates
- First principle calculations for chemisorption and molecular reactivity at surfaces
- Catalytic reaction pathways for molecules from DFT calculations
- Modeling grafted complexes or clusters on oxide surfaces
- Simulation of catalytic surfaces and particles in realistic temperature and pressure conditions
- Modeling of electrocatalysis and photocatalysis; applications to fuel cells, CO₂ reduction and water splitting.

5- Publications

- 292 publications in refereed journals (with 1 Science, 1 Nature Chem., 1 ACS Cent. Sci., 17 JACS, 9 Angew. Chem., 14 ACS Catalysis, 22 J. Catal., 2 Chem. Sci., 3 Phys. Rev. Lett., 2 Chem. Rev., 24 Phys. Rev. B, 15 PCCP, 4 Chem Cat Chem, 9 Chem. Phys. Lett , 55 J. Phys. Chem., 5 Organomet., 36 Surface Science)
- 13 book chapters
- 4 patents
- h factor = 56 (ref WOS) or 62 (Google Scholar); > 10000 citations
- >100 invited lectures at conferences

Selected recent publications

- 1) Federico Calle-Vallejo, David Loffreda, Marc T. M. Koper and Philippe Sautet
Introducing structural sensitivity into scaling relations between adsorption energies by means of coordination numbers
Nature Chem. 7, 403-410 (2015)
- 2) Aleix Comas-Vives, Maxence Valla, Christophe Copéret and Philippe Sautet
Cooperativity between Al-sites promotes H-transfer and carbon-carbon bond formation upon dimethylether activation on alumina
ACS Cent. Sci., 1, 313-319 (2015)
- 3) Federico Calle-Vallejo, Jakub Tymoczko, Viktor Colic, Quang Huy Vu, Marcus D. Pohl, Karina Morgenstern, David Loffreda, Philippe Sautet, Wolfgang Schuhmann, Aliaksandr S. Bandarenka
Finding optimal surface sites on heterogeneous catalysts by counting nearest neighbors
Science, 350, 185-189 (2015)

4) Carine Michel, Jérémie Zaffran, Joanna Matras-Michalska, Marcin Jedrzejczyk, Agnieszka M. Ruppert, Jacek Grams, and Philippe Sautet
Role of water on metal catalyst performance for ketone hydrogenation. A joint experimental and theoretical study on levulinic acid conversion into gamma-valerolactone
Chem. Comm. 50, 12450 (2014)

4) Federico Calle-Vallejo, José I. Martínez, Juan M. García-Lastra, Philippe Sautet and David Loffreda
Fast prediction of adsorption properties for platinum nanocatalysts with generalized coordination numbers
Angew. Chem. Int. Ed. 53, 8316-8319 (2014)

5) Florian Göttl, Rosa E. Bulo, Jürgen Hafner, Philippe Sautet
What makes copper-exchanged SSZ-13 zeolite efficient at cleaning car exhaust gases?
J. Phys. Chem. Lett. 4, 2244-2249 (2013)

6- Teaching

- UCLA, Graduate Thermodynamics, CH ENG 200, Fall quarter 2016
- Ecole Normale supérieure de Lyon, Molecular orbitals and application to chemical reactivity, course at master level, since 2011
- Professor at Ecole Polytechnique, Paris (in addition to my research position at CNRS), theoretical chemistry and applications to organic and organometallic chemistry, course and exercises at bachelor and master level, 1993 - 2005
- University of Lyon, Quantum chemistry applied to catalysis (solids, surfaces, and surface chemistry), course at master level, since 1993
- Molecular orbitals in organic and organometallic chemistry, course at master level, Ecole Normale Supérieure de Lyon, 1987 – 1991
- Responsible of the master of Chemistry, specialty catalysis and physical chemistry, University Claude-Bernard Lyon 1 and Ecole Normale Supérieure, 2004-2008
- Coordinator of the 2nd year of the master of matter sciences, option Chemistry, Ecole Normale Supérieure, 2004-2006

7- Supervision of students and post-doctoral researchers

- 24 PhD thesis defended under my supervision, 5 in preparation. Among the 24 doctors, 7 are now professors in the French university system, 2 full professors, 8 researchers (CNRS, IFPEN, industry), 2 teachers and 5 post-doctoral researchers
- 14 Post-doctoral researchers.

8- Funded projects

By industry

- Total 2014-2017 « acetylene selective hydrogenation including green-oil formation using combined DFT and kinetic Monte Carlo modeling » 1 PhD funded.
- IFPEN 2014-2017 « Catalytic activity of bimetallic clusters supported on gamma alumina » 1 PhD funded.
- Solvay 2013-2016, "Selective amination of alcohols" 1 PhD funded
- Solvay, 2013-2014, "Catalytic transformation of CO₂" 1 post-doctoral researcher funded
- Total / Hutchinson, 2011-2013, "Molecular dynamics simulation in the polymer

transformation industry" (1 post-doctorant)

-Rhodia, 2011-2013, "mechanisms in oxidation catalysis" 1 post-doctoral researcher funded

-IFP, 2008-2012, "Modeling of reforming catalysts", 1 PhD funded

- Total, 2007-2008, « Molecular modeling of organogelators for bitumen applications», 1 post-doctoral researcher funded

- Total 2004-2005 « theoretical modeling of the interaction between surfactant molecules and a surface of silica », 1 post-doctoral researcher funded

- IFP, 2003-2006, "Modeling metallic clusters on gamma alumina", 1 PhD funded

- IFP, 2000-2006, "Structure of gamma alumina, support of catalysts", 1 PhD funded

- EDF, 2001 « Order N calculations with Siesta in Fe and Zr".

International projects

- KAUST university (Saudi Arabia) « Carbon-neutral hydrogen production: water splitting ». Co-PI with Kazuhito Takanabe, 2014-2020. Funding of a post-doctoral researcher for 6 years

- ANR-FNS (France-Switzerland) 2014-2018 MASCAT Monitoring active sites of metathesis catalysts: a combined operando spectroscopy and computational approach, with ETH Zurich and Paul Scherrer Institute. 1 Post-doc funded

- ANR-NSF (France-USA) MUSIC, Multiscale Simulations of Bifunctional Catalysis, 2014-2018, with U San Digo et U Delaware. 1 PhD student and 1 Post-doc funded

- « Funcat » international laboratory between CNRS, ENS de Lyon and Ottawa university. 2013-2016. Student and researcher travels funded.

- Participation to the projects of the E2P2 laboratory (Eco-efficient processes and products) in Shanghai, Solvay-CNRS-ENS Lyon-ECNU, 2011-2015.

- KAUST university (Saudi Arabia) CADENCED « Computer Assisted Discovery and Elucidation of Catalysts for Economic Development of Saudi Arabia » including IFP, CNRS and ENS Lyon. 2009-2013. For the laboratory, it was associated with the funding of 10 years of postdoctoral researcher.

Projects funded by European Community

- PUMA-MIND « modeling PEM Fuel Cells», 2013-2016, 2 PDA funded

- Initial Training Network « Small » Surfaces for molecular recognition at the atomic level (2009-2012), 2 PhD funded

- Excellence network IDECAT « Integrated design of catalytic nanomaterials for a sustainable production » (2006-2010)

- Concerted action CONCORDE on oxidation catalysis: 2003-2005

- "Marie-Curie" training site "modeling heterogeneous catalysis" 2001-2004

French funded projects (ANR is the French funding agency)

- ANR SHAPES, New selective amination processes for the synthesis of biosourced monomers 2013-2016 (collaboration with Solvay and Lille university), 1PDA funded

- ANR GALAC, Synthesis of acrylic acid from glycerol via lactic acid, 2011-2014, 1 PhD funded

- ANR DYQUMA, Theoretical study of the dynamics of adsorbed molecules, 2011-2013, 1PDA funded

- ANR « SIRE, Simulation of reactivity at interfaces » 2007-2010, 2 PDA funded

- DEISA-DECI 2009, « Simulation of reactivity at interfaces », 1 200 000 hours CPU.

- ANR « ECLAT nanotubes for low consumption LCD screens » 2007-2009
- ANR « MéthanoX, Application of organometallic chemistry to selective oxidation of methane in methanol » 2007-2009, 1 PDA
- Meso-computing, "Electronic structure and dynamics of complex systems", 1998-2002, 150 K€ in computing equipment

9- Services

Administrative services

- Director of the "Institut de Chimie de Lyon", FR CNRS 3023, 2007-2015 (1000 persons). This Institute is the cluster of all the chemistry research laboratories in Lyon. Under my guidance the Institute obtained in 2015 a **funding of 12 M€** for equipment for the discovery of new catalysts and polymer materials and for their scale-up from lab to industry scale.
- Responsible of the international laboratory "Fundamental catalysis for green chemistry: From well-defined active sites to mechanistic explorations" between the CNRS, the ENS de Lyon and the university of Ottawa (2013-...)
- Chair of the Chemistry section at the French Academy of Science (2014-...)
- Director of the « Laboratoire de Chimie », UMR CNRS, Ecole Normale Supérieure de Lyon, France, 2003-2010 (90 persons)
- Member of the scientific council of the "Ecole Normale Supérieure" of Lyon 2000-2006, 2009-2010.
- Member of the administration council of the "Ecole Normale Supérieure" of Lyon 2006-2009, 2010-2013.
- Member of the council of the Physical-Chemistry division of the French Chemical Society.

Panel Services

- Chairman of the Panel PE4 (Physical and Analytical Chemistry) of the European Research Council (2011-2014)
- Member of the Panel PE4 (Physical and Analytical Chemistry) of the European Research Council (2008-2010)
- Nominated member of the French National Council of the Universities 1999-2011
- Member of the scientific council of IFPEN (French Institute of Petroleum and new energies) (2009-...)
- Member of the scientific council of GDF-Suez (Energy company in Europe) (2013-...)
- Expert for AERES (French research evaluation organization) and ANR (French funding agency)
- Expert evaluator for the "Improving Human Capital" program of the EC, under the FP5 and FP6 framework
- Member of the program committee of IDRIS (Computing Institute of CNRS), CNRS 1998-2008.

Editorial activities

- Associate Editor of the journal "ACS Catalysis" published by the American Chemical Society (since 2012)

- Member of the editorial board of the New journal of Chemistry (2002-2005), the Journal of Molecular Catalysis (2003-2007), Surface Science (2007-...), ChemCatChem (2009-2013), Catalysis Letters (2009-...) and Topics in Catalysis (2009-...)
- Associate Editor of the journal « Catalysts and Catalyzed Reactions » 2002-2004

10- Organization of Conferences and workshops

- Symposium "Computational Chemistry across Catalysis", in the ACS congress in San Diego (March 2016)
- RCTF (meeting of the French speaking theoretical chemists), Lyon, May 2016.
- President of the international conference EUROPACAT, European Conference on Catalysis, September 2013, Lyon (1700 participants)
- International congress Inmother 2012 "Industrial use of molecular thermodynamics", Lyon, Mars 2012
- International symposium "Tomorrow toward a selected Chemistry: Chemistry, keystone of sustainable Energy", Lyon, October 2011
- International summer school « Computational Catalysis and materials science », Lyon, May 2010
- CECAM workshop «Molecular recognition and selectivity at surfaces », October 2007
- International summer school « Computational Catalysis and materials science », Porquerolles, September 2007
- Summer School on Theoretical Physical Chemistry, Aussois, October 2001
- International conference « Theoretical aspects of heterogeneous catalysis, CAT2000 », La Colle sur Loup, Mai 2000.

11- International visits (of duration at least 1 month)

- Lawrence Berkeley National Laboratory (Berkeley, USA), September 1991- September 1992
- Theoretical Chemistry Laboratory, Free University of Amsterdam, September 1993
- Lawrence Berkeley National Laboratory (Berkeley, USA), July-August 1994
- Lawrence Berkeley National Laboratory (Berkeley, USA), June-August 1997
- Schuit Institute, University of Eindhoven, March 1999
- Center for Catalysis Research and Innovation, University of Ottawa, July 2013
- ETH Zürich, Department of Inorganic Chemistry, January-March 2016