Key role of the joint experimental-theoretical approach in the understanding of reactivity in the field of homogeneous catalysis

Karinne Miqueu
CNRS/University PAU & PAYS ADOUR

Jueves, 28 de noviembre
12:00 h
Sala de Grados de la Facultad de Ciencias

CICLO CONFERENCIAS **ISQCH** 2019

Instituto de Síntesis Química y Catálisis Homogénea

Facultad de Ciencias, Universidad de Zaragoza - CSIC
C/ Pedro Cerbuna, 12. Zaragoza 50009. Spain

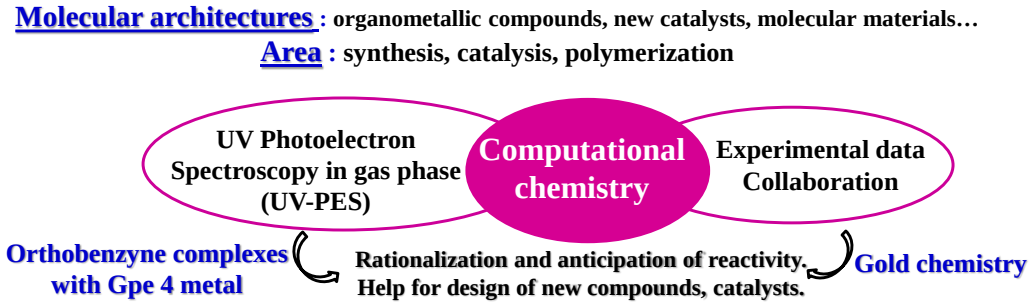
Facultad de Ciencias Universidad Zaragoza

Key role of the joint experimental-theoretical approach in the understanding of reactivity in the field of homogeneous catalysis

Karinne Miqueu
CNRS/University Pau & Pays Adour, IPREM UMR 5254, Helioparc 2 avenue P. Angot. F-64053 Pau, France. e-mail : karinne.miqueu@univ-pau.fr

Nowadays, computational chemistry is involved in nearly every area of chemistry (molecular chemistry, materials, life sciences ….) and has become an essential tool, just like classical laboratory techniques, for mechanistic understanding of gas or solution-phase chemical reactions. The joint experimental-theoretical approach plays an increasingly larger role to solve a wide array of organic/organometallic problems and a thorough understanding of the reactivity has been gained thanks to this synergy, especially in polymerization and in catalysis areas. The description of the electronic structure and new bonding situations as well as the investigation of the different plausible reaction pathways and the analysis of the limiting and determining steps provide crucial mechanistic insights allowing to have a better understanding of the reactivity. Moreover, modern computational methods also give relatively accurate and fast results which make them a suitable tool for the prediction of properties, reaction feasibility, selectivity… and can be helpful in the design of new reactions and catalysts.

To demonstrate the fruitful interplay between experiment and theory, different examples will be presented more specifically in the field of homogeneous catalysis. One project will concern the rationalization and understanding of reactivity of gold complexes[1] and the other one the characterization of short life orthobenzyne complexes with early metals by coupling Flash Vacuum Thermolysis with an original spectroscopy - UV-Photoelectron Spectroscopy in gas phase - and DFT calculations.[2]



[1] a) see for instance : M. Rigoulet, S. Massou, E.- D. Sosa-Carrizo, M. Ladeira, A. Amgoune, K. Miqueu, D. Bourissou. PNAS, *116 (1,2),* **2019**, 46. b) J. Serra, P. Font, E.- D. Sosa Carrizo, S. Mallet-Ladeira, S. Massou, T. Parella, K. Miqueu, A. Amgoune, X. Ribas, D. Bourissou. *Chemical Sciences*, 9, **2018**, 3932. c) F. Rekhroukh, C. Blons, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou. *Chemical Sciences*, 8 (6), **2017**, 4539. d) F. Rekhroukh, L. Estévez, C. Bijani, K. Miqueu, A. Amgoune, D. Bourissou. *Ang. Chem. Int. Ed. Engl.*, 55(10), **2016,** 3414. e) F. Rekhroukh, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou. *J. Am. Chem. Soc.*, *138*(36), **2016**, 11920. f) A. Zeineddine, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou, *J. Am. Chem.Soc.*, *136* (42), **2014**, 14654.

[2] a) S. Labat, K. Miqueu, J.-M. Sotiropoulos, P. Baylère, G. Pfister-Guillouzo, N. -H. Tran-Huy, F. Mathey, *EJIC*, **2014**, 1694. b) K. Miqueu, S. Labat, E. -D. Sosa Carrizo, J. -M. Sotiropoulos. *EJIC*, **2018**, 2717.

Karinne Miqueu – CNRS Senior Researcher
e-mail : karinne.miqueu@univ-pau.fr
Institution: **CNRS/University PAU & PAYS ADOUR**
Research at **IPREM UMR 5254, Hélioparc, 2 avenue P. Angot, 64053 Pau cedex 09. France.**
http://www.iprem.univ-pau.fr . http://orcid.org/0000-0002-5960-1877.

Titles, Degrees and Professional Experience

1996-2000 **Assistant Professor**- University Pau & Pays Adour
Janv. 2000 **PhD in Physical-Chemistry** at Univ. Pau & Pays Adour. Laboratory of "Chimie Théorique et Physico-Chimie Moléculaire". Supervisor G. Pfister-Guillouzo.
2000-2001 **Post-Doctoral position**. Laboratory of Chemical Physics, Southampton (England). Reactive intermediates in gas phase with experimental and theoretical methods. Supervisor J.-M. Dyke.
2001-2002 **Post-Doctoral position**. Laboratory of "Hétérochimie Fondamentale et Appliquée", UMR 5069, Toulouse (France). Carbene chemistry. Supervisor G. Bertrand.
2002-2014 **CNRS Assistant Researcher** – Univ. Pau & Pays Adour. IPREM, UMR CNRS 5254.
2011 « Habilitation à Diriger des Recherches » (HDR) – Univ. Pau & Pays Adour.
Since 2014 **CNRS Senior Researcher** – Univ. Pau & Pays Adour. IPREM.

Research interests

Computational Chemistry – UV Photoelectron Spectroscopy in gas phase – Joint experimental-theoretical approach.
Main group chemistry – Organometallic chemistry – Coordination chemistry – Reactive intermediates
Electronic structure – Spectroscopic properties – New bonding situation – Reactivity
Mechanisms – Catalytic reaction pathways – Polymerization reaction pathways – Homogeneous catalysis

Scientific contributions - Award

- **1996-2019** Co-author of ***111*** publications in peer-review journals
  46 oral communications (10 invited conferences)
- ***H factor = 32*** *– 3141 citations – 2876 without self-citations (source: Web of Science - September 2019)*
- **Award** : Bronze medal of CNRS in **2010**

Other activities

Teaching : ~ 30 h of lectures by year at 3rd year level in Physical-Chemistry since 2012. Univ. of Anglet.
Member of the CoNRS, section 12 (2017-2021).
Member of the Scientific Council Univ. Pau & Pays Adour (2016-2020).
Treasurer French Chemical Society – Section Aquitaine (2015-2019). Member since 2005.
Supervision : 4 PhD, 6 post-doctoral fellows (duration of each contract : 2-3 years). Reviewing activities of 9 PhD and 1 Habilitation.

Selection of some publications since 2014

1. Catalytic Au(I)/Au(III) arylation with the hemilabile MeDalphos ligand: unusual selectivity for electron-rich iodoarenes and efficient application to indoles. J. Rodriguez, A. Zeineddine, E.- D. Sosa Carrizo, K. Miqueu, N. Saffon Merceron, A. Amgoune, D. Bourissou. *Chemical Sciences, 10,* **2019,** 7183-7192.
2. Evidence for genuine hydrogen bonding in gold(I) complexes. M. Rigoulet, S. Massou, E. -D. Sosa-Carrizo, S. Mallet-Ladeira, A. Amgoune, K. Miqueu, D. Bourissou. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*, *16(1)*, **2019**, 46-51.
3. Cyclometalated Gold(III) Complexes: Noticeable Differences between (N,C) and (P,C) Ligands in Migratory Insertion. J. Serra, P. Font, E.- D. Sosa Carrizo, S. Mallet-Ladeira, S. Massou, T. Parella, K. Miqueu, A. Amgoune, X. Ribas, D. Bourissou. *Chemical Sciences,* 9, **2018**, 3932-3940.
5. Short-lived orthobenzyne complexes with early transition metals of group IV. First direct characterization and electronic cartography by coupling FVT/ UV-PES and calculations. K. Miqueu, S. Labat, E.- D. Sosa Carrizo, J.- M. Sotiropoulos. *European Journal Inorganic Chemistry*, **2018,** 2717-2729.
6. Rational development of catalytic Au(I)/Au(III) arylation involving mild oxidative addition of aryl halides. A. Zeineddine, L. Estevez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou. *Nature Communications*, 8(1), **2017**, Article number 565.
7. Gold(III)-arene complexes by insertion of olefins into gold-aryl bonds. F. Rekhroukh, C. Blons, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou. *Chemical Sciences,* 8 (6)*,* **2017,** 4539-4545.

8. Experimental and theoretical evidence for an agostic interaction in a Gold(III) complex. F. Rekhroukh, L. Estévez, C. Bijani, K. Miqueu, A. Amgoune, D. Bourissou. *Ang. Chem. Int. Ed. Engl.,* 55(10)*,* **2016,** 3414-3418.
9. Coordination-Insertion of Norbornene at Gold: A Mechanistic Study. F. Rekhroukh, L. Estévez, C. Bijani, K. Miqueu, A. Amgoune, D. Bourissou. *Organometallics,* 35 (7), **2016,** 995–1001.
10. β-Hydride Elimination at Low-Coordinate Gold(III) Centers. F. Rekhroukh, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D. Bourissou. *Journal of the American Chemical Society, 138*(36), **2016,** 11920-11929.
11. Facile oxidative addition of aryl iodides to Gold(I) by ligand design: Bending turns on reactivity. M. Joost, A. Zeineddine, L. Estévez, S. Mallet-Ladeira, K. Miqueu, A. Amgoune, D.Bourissou, *Journal of the American Chemical Society*, *136* (42), **2014**, 14654-14657.
12. A Contribution to the Direct Observation of Transient Phosphanylidene Complexes [RP=W(CO)5, (R: Me, Ph)]: A Revisited Approach to Their Electronic Structure by UV Photoelectron Spectroscopy. S. Labat, K. Miqueu, J.- M. Sotiropoulos, P. Baylère, G. Pfister-Guillouzo, N.- H. Tran-Huy, F. Mathey, *European Journal of Inorganic Chemistry*, **2014**, 1694-1705.