

Hélène GERARD

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Education, career and positions

2009 - ...: Full Professor at Sorbonne Université - Laboratoire de Chimie Théorique (UMR 7616)

2007: Habilitation (HDR) - Université Pierre et Marie Curie – Paris 6

2001-2009: Assistant Professor at UPMC – Paris 6 - Laboratoire de Chimie Théorique (UMR 7616)

2001: Post-doctoral training at Bloomington University, Indiana, USA. Supervision Pr. G. J. Martyna

February 2000: doctoral training at Bloomington University, Indiana, USA. Supervision Pr. E.R.

Davidson and K.G. Caulton

1998-2001: Ph D in Theoretical Chemistry at University Montpellier II under direction of O. Eisenstein

Current research interest

Theoretical studies (reaction mechanisms and potential surfaces) of structure, reactivity and properties of molecular compounds in complex reactive microenvironment

Problematic of interest : association and self-assembly processes, electron transfer reactions

Major responsibilities

- Since September 2022: Co-responsible for the Physical and Theoretical Analytical Chemistry speciality of the **Sorbonne University Master of Chemistry**

- Since January 2019: animation of the **scientific team " Inorganic, Organometallic and Organic Chemistry "** of the LCT

- Since March 2017: Elected member of the **UFR Chemistry Council** – 926. In this context: equality and anti-discrimination referent, participation and chairing of recruiting and advancement committees

- 2011-2018: **Director of the Doctoral School 388** Physical Chemistry and Analytical Chemistry of Paris Centre (about 300 students). In this context and afterwards: outsider member of other doctoral school boards, expert in charge of the HCERES evaluation for the doctoral schools and/or the doctoral college (2019, 2020-22 : presidency) and since 2018 - ... : teaching (2 sessions / year) scientific integrity for ED 388

- 2012-2016: **Elected member of the Administration Council** of UPMC-Paris 06. In this context and afterwards: appointed member (2012-16, external personality) of the Board of Directors of the University Paris Sorbonne - Paris 04, member (2012-16) of the disciplinary section "users", in charge of the **"equality" mission for the President** of UPMC (2016-18).

- 2008-2016: Coordination of the theoretical partner of various (financed) ANR projects : ANR-12-BS07-0009-01 (SCATE), ANR-09-BLAN-0089-01 (COPENOL), ANR-07-BLAN-0294-01 (AggregAte)

Scientific production

72 publications (h index = 23), 2 book chapters, 2 scientific mediation articles, 1 patent.

Director of 3 finalized PhD students plus 2 ongoing ones.

Sample of recent publications

"Cu(I)-Assisted Addition of Li- or Zn-Organometallics to Carbonyl Compounds: Learning from Analogies and Differences Between Intermediates and Transition States", S. Halbert, H. Gérard, *Top. Catal.* **2022**, *65*, 481-492. DOI : 10.1007/s11244-021-01551-9.

"Intertwined Analytical, Experimental and Theoretical Studies on the formation and structure of a Copper dienolate.", B. Lecachey, L. Palais, B. de Courcy, S. Bouauli, M. Durandetti, H. Oulyadi, A. Harisson-Marchand, J. Maddaluno, H. Gérard, E. Vrancken, J.-M. Campagne, *Chem. Eur. J.* **2021**, *27*, 7942-7950. DOI : 10.1002/chem.202100596.

"Triggering electron transfer in Co(I) dimers: computational evidences for a reversible disproportionation mechanism" M. Guillaumont, I. Furré, J. Pilmé, S. Halbert, H. Gérard, *ChemPhysChem* **2021**, *22*, 788–795. DOI: 10.1002/cphc.202000965.