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i-CLeHS

Theoretical Chemistry and  
Modeling Team

## Prof. Carlo Adamo Curriculum Vitae



## Career Outlines

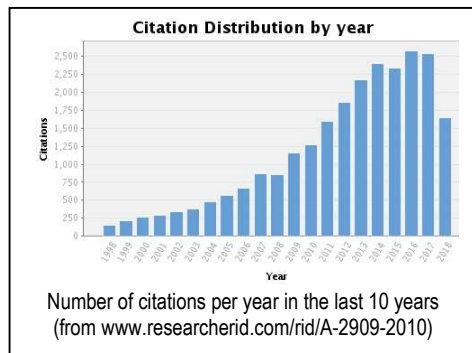
I received my **PhD degree** in Theoretical Chemistry from the University "Federico II" of Naples in 1994. In 1993, before the end of PhD, I was hired as **tenured assistant professor** by the University of Basilicata (Potenza, Italy) as assistant professor. From October 1996 to September 1997 I was on a **sabbatical year** at the Laboratoire de Reconnaissance Ionique of the CEA-Grenoble, in charge of the development of research activity concerning the first-principles modeling of lanthanide and actinide complexes. Since 1998, this collaboration produced 15 papers and 2 co-directed PhD thesis (Valentina Vetere 2001 et Laurence Petit 2007). I also worked on the development of new DFT functionals and, thanks to this latter activity, I was included as co-author of the computer code Gaussian ([www.gaussian.com](http://www.gaussian.com)) since 1998.

During the academic years 1997-1998 and 1998-1999 I was a professor with a temporary appointment at the University of Naples for the course of Molecular Modelling (Faculty of Pharmacology, 40h, 15 students) and Physical Chemistry (Faculty of Agronomy, 60h, 100 students). In 1999 I was invited by prof. Scuseria at Rice University to collaborate on a project concerning DFT and TD-DFT. 8 articles have been published within this collaboration.

In September 2000 I was nominated as **associate professor** at ENSCP and upon my arrival in Paris I was in charge for the development of both research and teaching activities in the Institute. In 2001, with the hiring of Laurent Joubert (now professor at the University of Rouen) I created the group of Theoretical Chemistry and Modelling which now, after 16 years, is composed of 8 permanents and about 20 non-permanents (PhD students and Post-doctoral fellows). This group, still under my responsibility, is one of the most productive at our Institute, having published more than 200 articles in the last 5 years and having raised a significant amount of research funds, including an ERC Consolidator grant (PI Dr. Ilaria Ciofini). Concerning the teaching activities, I introduced courses in Computational/Theoretical Chemistry and Molecular Modeling in the cursus of the ENSCP students, thus initiating young French chemical engineers to the theory and practice of these fields also in industrial environments.

All these activities have been well recognized by the community and since 2000 I have quickly climbed all of the academic career steps: full professor (**professeur première classe** 2004), chair (**professeur classe exceptionnelle**, 1<sup>er</sup> echelon 2011, 2<sup>ème</sup> echelon 2016).

In 2001 and 2005 I was an invited professor at the Pontificia Universidad Catolica de Chile (Santiago, Chili) for 2 months and then, in 2009, an invited researcher for 3 months at the Institute of Mathematics and its Applications of the University of Minnesota.



Year 2011 represents a turning point in my career : I was promoted to the chair of theoretical chemistry (**professeur de classe exceptionnelle**, 1<sup>er</sup> échelon) and I was admitted as **senior member** at the Institut Universitaire de France (IUF), the third senior theoretical chemists since the creation of IUF and the only one still in activity at the time of nomination. I was nominated a **second time** in 2018.

**From 2014 to 2016** I had a collaboration with the Italian Institute of Technology ([www.iit.it](http://www.iit.it)), where I spent 3 months/year (6 months in total) as visiting researcher. There, I was in charge of 2 post-doctoral fellowships (Marika Savarese and Eric Brémont)

and the results of our research was published in 16 articles and presented as in 8 oral communications at international congresses.

During my career I have published **380** articles in peer-reviewed journals, which received more than **24000 citations** (an average of 63 citations per article). Of these articles, 2 received more than 2000 citations and 36 more than 100 citations. My **h-factor is 65** (source WOS 24/04/2018). 10 of my articles, published in the last 10 years, are classified as highly cited in Essential Science Indicators<sup>SM</sup> (ESI) by InCites, that is they are in the top 1%. According to InCites "Highly Cited Papers are considered to be indicators of scientific excellence and top performance and can be used to benchmark research performance against field baselines worldwide".

In 2009 I was nominated in the **Advisory Board of Physical Chemistry Chemical Physics**, the journal of the Royal Chemical Society with the highest impact factor in Physical Chemistry. Since 2015, I am **Editor in Chief of Theoretical Chemistry Accounts**, the oldest journal dedicated to Theoretical Chemistry, published since 1962 by Springer. In this role, I handle about 400 manuscripts per year.

I was involved in several organizing and scientific committees of national and international conferences. Among others, I would like to mention the *Rencontre de Chimistes Théoriciens Francophones*, biannual national meeting

in Theoretical chemistry, where I have been in the scientific committee since 2006 and member of the organizing committee for the 2014 edition and the *International Conference on the Applications of Density Functional Theory in Chemistry and Physics* (DFT09, 2009), the international meeting which bring together about 450 scientists working in the field of DFT. More recently, I participated in the scientific committee of *10<sup>th</sup> Congress of the World Association of Theoretical and Computational Chemists* (WATOC 2014, Santiago du Chile), which saw the participation of about 800 theoretical chemists, and to the organization of the XLIII Congrès des Chimistes Théoriciens d'Expression Latine Paris (France) 3-7 July 2017. This latter event is, together with the Sanibel Symposia, the oldest congress in Theoretical Chemistry, the first edition dating back to 1962. The 2017 edition, was attended by 170 participants coming from Europe, Africa and Americas.

I had also several activities concerning the evaluation of research quality. Among others, in 2015 I was nominated by the Italian Ministry of Education, Universities and Research (MIUR) in the panel for the evaluation of the research (panel **Valutazione Qualità Ricerca VQR – GEV03**, 22 members in total). This panel evaluates the research activities in Chemistry carried out by all the Italian Universities, during the period 2011-2014. I actively participated in the activities of the panel the last two years, including several meeting at MIUR in Rome, and I handled about 500 scientific products (mainly research articles). The final meeting of the panel was held on 14/10/2016.

From 2012 to 2018 I was member of the PE5 panel (Synthetic Chemistry and Materials) of the European Research Council (ERC) for the **ERC-StG** grants (call 2012, 2013, 2015 & 2017). As panel member, I participated to the remote evaluation of the projects (around 35 project/yr) and to the interviews in Brussels (1 week, around 50 candidate/yr).

Since 1<sup>st</sup> January 2019, I am the head of the Institute of Chemistry for Life and Health Sciences, a laboratory of CNRS and ENSCP. This lab is composed by 3 experimental and 1 theoretical teams, for a total of 26 permanents and about 50 non-permanent staff (post-docs and PhD students)

#### **Scientific production**

- More than 380 papers in international peer-reviewed journals (see [www.researcherid.com/rid/A-2909-2010](http://www.researcherid.com/rid/A-2909-2010))
- h-factor = 67, with more than 25 000 citations in Web of Science (2 papers with more than 2000 citations, 40 with more than 100 citations, WoS 13/08/2018)
- 74 invited lectures and 164 communications at national and international congresses
- Co-author of the computer code Gaussian since 1998 ([www.gaussian.com](http://www.gaussian.com))

#### **Editorial activities**

- Editor-in-Chief of Theoretical Chemistry Accounts, (Springer, IF=1.8) since 2015
- Advisory Board of Physical Chemistry Chemical Physics, Royal Society of Chemistry since 2009
- Editor of Molecules (MDPI, IF 2.86) since 2016
- Editor of Central European Journal of Chemistry (De Gruyter Open, IF 1.09) 2013-2015
- Guest Editor for Theoretical Chemistry Accounts, International Journal Quantum Chemistry, Physical Chemistry Chemical Physics, Journal of Molecular Modeling

#### **Awards**

2011 - 2016 Senior member of the Institut Universitaire de France, Paris, France ([www.iufrance.fr](http://www.iufrance.fr))  
2018 - 2023 Senior member of the Institut Universitaire de France, Paris, France

The Institut Universitaire de France (IUF) is a service of the Ministry of Higher Education and University that distinguishes each year a small number of university professors for their research excellence, as evidenced by their international recognition. Only 2% of French university professors have been distinguished by the IUF since its creation in 1991. In 2011, I was the third senior theoretical chemist admitted to IUF and the only one still in activity. I am the only theoretical chemist who has been nominated for a second time.

#### **Research-related activities**

- Head of the Group Theoretical Chemistry and Modeling, Institut de Recherche de Chimie Paris. The Group is composed by 5 permanents and 10 non-permanents (PhDs and post-docs)
- Member nominated of the Scientific Council of Paris Science et Lettre (PSL) University (2012-2015)
- Elected member of the Scientific council of ENSCP (2001-2005 & 2011-2015)

- Member of the Scientific Council of the PhD school in Material Science, joint PhD school between the University of Palermo and University of Catania (Italy), 2012-2013
- Member of the Scientific Council of the PhD school in Chemistry, Scuola Normale Superiore (Pisa, Italy), 2014 onwards
- Invited Researcher at: CEA-Grenoble, 1996-1997, 1998; Rice University, Houston (USA) 1999; University of Santiago (Chili) 2001, 2005; University Joseph Fourier, Grenoble (France) 2000; University of Naples (Italy), 2005; Minnesota University, Minneapolis (USA) 2009;
- Invited Professor, International School for Advanced Studies (SISSA), Trieste (Italy), April 2006, course and practicals on DFT (42h)
- Invited Professor, German Research School for Simulation Sciences, Jülich (Germany), March 2011, course on DFT (22h)
- Invited Professor, University of Palermo, Palermo (Italy), October and November 2014, course on modeling devices for renewable energies, course and practicals (59h)
- External collaborator of the Italian Institute of Technology, Genoa (Italy) 2014-2016.

### Networks

- Co-founder and Member of the Management Committee of the French Network of Theoretical Chemists (GdR n. 3333, 2006-2016)
- Management Committee of CNRS Research Group (GdR) « Méthodes corrélées pour la structure électronique » (Correl) (2011-2013 and 201-2018)
- Management Committee of the computer center MESO@PSL of PSL Research University since its creation in 2010
- Member of the international CNRS Research Group (GDRI) Sino-French Theoretical Chemistry (2014-2017)
- Management Committee of the Ile-de-France and Lorraine area node (CECAM-FR-MOSER) of the Centre Européen de Calcul Atomique et Moléculaire (CECAM) since its creation in 2010
- INSERM panel on *Reproductive toxicity*, nominated expert in charge of the molecule-receptor modelling (2009-2011)
- ANR-CNRS join panel « pro-REACH » (2008-2009), nominated expert in charge of modelling approaches within the REACH European legislation
- Coordinator of a working group « Chemistry for the panel « Production Grid » on computer grids, Institut de Grille CNRS (2009)

### Conferences

Committee Member in 27 national or international congresses. The most recent ones:

- 10<sup>th</sup> Congress of the World Association of Theoretical and Computational Chemists (WATOC), 5-10 October 2014, Santiago (Chile), scientific committee, 800 participants
- 14<sup>ème</sup> Rencontre des Chimistes Théoriciens Francophones, 1-4 July 2014, Paris (France), organizing and scientific committees, 200 participants
- 7th Symposium on Theoretical Biophysics (TheoBio 2015), Cagliari, Italy, 8-12 June 2015, scientific committee, 120 participants.
- Theory and Applications of Computational Chemistry 2016 (TACC 2016), Seattle (USA) 28 August- 2 September 2016, International Advisory Committee, 250 participants
- XLIII Congrès des Chimistes Théoriciens d'Expression Latine Paris (France) 3-7 July 2017, organizing committee, 170 participants

### Funds

#### National agencies

- 1 ACI Jeune Chercheur **CNRS**
- 6 **ANR** projects : pre-THECES (2006) ; Hétéro-eau (2007-2009) ; NEXUS (2008-2010), PREDIMOL (2010-2012), DinFDFT (2010-2012), E-Storic (2014-2017).

#### European agencies

- FP7 Project : *New materials for hydrogen powered mobile applications* - HYPOMAP (FP/-NMP-2008-CT233482) (2009-2012);
- FP7 Project *Computer simulations of thermally excited molecules and materials by first principles* - TEMM1P (PIRSES-GA-2011-295172) (2012-2015) ;
- H2020 project: Supervisor of a Marie Skłodowska-Curie grant, call H2020-MSCA-IF-2014, project COMBPDCHEMOTHERAPY (n. 652999) PI :Dr. Marta Erminia Alberto (2015-2017)
- COST action D26 Integrative Computational Chemistry, member of the Working Groups d26-0013-02 et d26-0001-02 (2002-2007);
- COST action CM1002, Convergent Distributed Environment for Computational Spectroscopy, French representative in the management committee and responsible of the Working Groups 1 (Development of multiscale approaches for computational spectroscopy) (2010-2013)

#### *Industrial contracts*

- Pechiney (2001), Institut Français du Pétrole (2006-2009) ; Institut National de l'Environnement Industriel et des risques (2007-2019) ; Sanofi-Aventis (2009-2012) ; L'Oréal (2012-2019)

#### **Evaluation of Research**

- Technical Committee 8 (Quantum Chemistry and Molecular Modelling) of the French high-performance computing agency (GENCI) (2014-onwards)
- Panel CHE (Chemistry) of the Research Executive Agency for the Marie Curie (FP7) et Marie Skłodowska-Curie (H2020) actions (2014-onwards)
- Panel "New Postdoctoral Programme Junior Leader la Caixa", La Caixa Bank, Barcellona, Spain (2018)
- Panel PE5 (Synthetic Chemistry and Materials) of the European Research Council (ERC) for the ERC-StG grants (2012, 2013, 2015, 2017)
- Panel of the Italian Ministry of Education, Universities and Research (MIUR) for the fund call PRIN 2012, in charge of the whole PE5 sector (Synthetic Chemistry and Materials, 2013)
- International Evaluation Committee of the "EPFL Fellows" program, Lausanne, Switzerland (2014-2017)
- Expert nominated by Italian Ministry of Education, Universities and Research (MIUR) for the evaluation of the quality in research, section Chemistry (panel **Valutazione Qualità Ricerca VQR – GEV03**), 22 members in total (2015-2016)
- Regular referee for several funding agencies, such as National Science Foundation (NSF), German Research Foundation (DFG), Swiss National Science Foundation (SNF), Netherlands Organisation of Scientific Research (NWO), Italian Ministry of University and Research (MIUR)

#### **Pedagogic and Administrative duties (last 5 years)**

##### *Pedagogic duties*

- Director of the Teaching Department « Methods in Mathematics and Informatics » of the ENSCP (2000-2014)
- Member of the Teaching Committee (Conseil de l'Enseignement et de la Vie Etudiante) of ENSCP (2000-2015)
- Board the PhD School in *Material Science*, joint PhD program between the university of Palermo and University of Catania (Italy) 2012-2014
- Board of the PhD School *Methods and Models for Molecular Sciences*, Scuola Normale Superiore, Pisa, (Italy), 2014-onwards (<http://phd.sns.it/metodi-e-modelli-per-le-scienze-molecolari/>)

##### *Administrative duties*

- Head of the Institute of Chemistry for Life and Health Sciences (i-CLeHS), 26 permanents and about 50 non-permanent staff (post-docs and PhD students).
- Head of the Research Group « Theoretical Chemistry and Modeling » Institut de Recherche Chimie Paris, UMR CNRS 8247 (2000-2018)
- Chef Operational Officer of ENSCP (directeur des opérations) in charge of the Chimie ParisTech infrastructure (2014-2016)
- Member of the Steering Board of ENSCP (6 members including Director, 2014-2016)

- Elected member of the Scientific Council of ENSCP (2011-2016)
- Nominated member of the Scientific Council of PSL Research University (2011-2015)