CURRICULUM VITÆ

Dr Pierre-François Loos (HDR)
CNRS researcher/chargé de recherche 1ère classe
Citizenship: French/Australian
Date of birth: 02/01/1982
email: loos@irsamc.ups-tlse.fr

IRSAMC
Laboratoire de Chimie et Physique Théoriques
UMR 5626, Université Paul Sabatier
Toulouse, France
http://www.irsamc.ups-tlse.fr/loos

Awards and Grants

2018	**Habilitation**, Université Paul Sabatier, Toulouse, France
2017 – 2018	**Visiting Fellow**, Australian National University, Canberra, Australia
2016	**Visiting Erskine Fellow**, University of Canterbury, Christchurch, New Zealand
2016	**Visiting Fellow**, University Paul Sabatier, Toulouse, France
2014 – 2016	**Discovery Project** grant from the Australian Research Council *"Accurate chemistry via resolution and quadrature"* ($330,000) DP140104071: Gill, Prof Peter M; Loos, Dr Pierre-Francois
2013 – 2015	**Discovery Early Career Researcher Award** from the Australian Research Council *"Thinking outside the box: spherical geometry in chemistry and physics"* ($365,219) DE130101441: Loos, Dr Pierre-Francois
2008	Best PhD dissertation in Molecular Physics and Chemistry (University of Nancy, 2008)
2005 – 2008	French government scholarship (*bourse MRT*) for PhD studies
2005 – 2008	Teaching assistant (University of Nancy, France)

Research Experiences

2017 –	**Chargé de recherche 1ère classe**, Centre National de la Recherche Scientifique (CNRS) Laboratoire de Chimie et Physique Quantiques, UMR5626, Universit'e Paul Sabatier, Toulouse, France
2016 – 2017	**Senior Lecturer** Group leader of the Mathematical and Theoretical Chemistry Group, Research School of Chemistry, The Australian National University, Canberra, Australia
2012 – 2015	**Australian Research Council Research Fellow** Discovery Early Career Researcher Award from the Australian Research Council, Group leader of the Mathematical and Theoretical Chemistry Group, Research School of Chemistry, The Australian National University, Canberra, Australia
2008 – 2012	**Postdoctoral Fellow in Theoretical Quantum Chemistry** — supervisor Prof Peter M. W. Gill — Theoretical Quantum Chemistry Group, Research School of Chemistry, The Australian National University, Canberra, Australia

2005 – 2008 **PhD Theoretical and Computational Chemistry**
— supervisor Prof Xavier Assfeld —
Theoretical Chemistry and Biochemistry Group (University of Nancy, France)
Development of a quantum chemistry method mixing several levels of theory: applications to the study of electronic states in macromolecular systems
Defence on 13th June 2008

Members of committee:
Prof A. Milet (University of Grenoble, France)
Prof Eric Perpète (University of Namur, Belgium)
Prof I. Tunon (University of Valencia, Spain)
Prof J.-L. Rivail (University of Nancy, France)
Prof C. Pouchan (University of Pau, France)
Prof X. Assfeld (University of Nancy, France)

2004 – 2005 **MSc Theoretical and Computational Chemistry**
— supervisor Prof Xavier Assfeld —
Theoretical Chemistry and Biochemistry Group (University of Nancy, France)
Optimization of localized orbitals within the local self-consistent field method

2003 – 2004 **MSc Soft Matter and Neutron Scatterring**
— supervisor Dr Julian Oberdisse —
Condensed Phase Dynamic Group (Montpellier, France)
Structural investigation of polymer-grafted-silica nanoparticles via small-angle neutron scattering: a Monte Carlo study

2002 – 2003 **BSc Theoretical and Computational Chemistry**
— supervisor Prof Xavier Assfeld —
Theoretical Chemistry and Biochemistry Group (University of Nancy, France)
Diabatic surfaces within the local self-consistent field method

Education

2000 – 2002 **Classes préparatoires** *PCSI/PC** at Lycée Henri Poincaré, Nancy, France
Intensive *post-baccalaureate* courses in mathematics, physics and chemistry

2002 – 2005 **BSc Physical Chemistry and MSc Theoretical Chemistry**
University of Nancy, France
2005: **Magistère Molecular Engineering**
2005: **MSc Theoretical and Computational Chemistry** (Mention très bien)
2004: **MSc Physical Chemistry** (Mention très bien)
2003: **BSc Physical Chemistry** (Mention très bien)

Oral communications

1. (Invited talk) August 2018, Molecular Electronic Structure (Metz, France)
   TBA

2. (Winter school lecture) January 2018, TCCM Winter School LTTC (Luchon, France)
   Theory and implementation of DFT-based methods

3. (Selected talk) August 2017, TouCAM 2017 (Toulouse, France)
   Dressing the CI matrix with explicit correlation

4. (Invited departmental seminar) September 2017, University of Basel (Basel, Switzerland)
   Expensive methods, cusps, integrals and other stuff
5. (Selected talk) August 2017, WATOC 2017 (Munich, Germany)
   Dressing the CI matrix with explicit correlation
6. (Invited talk) July 2017, 17th International Conference on Mathematical Methods in Science and Engineering (Cadiz, Spain)
   Electron-nucleus cusp dressing in single-determinant wave functions
7. (Invited departmental seminar) June 2017, University of Aix-Marseille (Marseille, France)
   Density-functional theory using finite uniform electron gases
8. (Invited talk) May 2017, Workshop on "Theory and applications of RPA and beyond in physics and chemistry", (Paris, France)
   Density-functional theory using finite uniform electron gases
9. (Invited departmental seminar) March 2017, University of Nantes (Nantes, France)
   Density-functional theory using finite uniform electron gases
10. (Invited talk) December 2016, Australian Symposium in Computational Chemistry (Perth, Australia)
    Excited states of Wigner crystals
11. (Invited talk) September 2016, Molecular Electronic Structure (Buenos Aires, Argentina)
    Three-electron integrals over Gaussian basis functions
12. (Invited talk) August 2016, New Zealand Institute of Chemistry Conference (Queenstown, New Zealand)
    How does Chemistry work in one dimension?
13. (Invited talk) July 2016, 16th International Conference on Mathematical Methods in Science and Engineering (Cadiz, Spain)
    Nodal surfaces in quasi-exactly solvable models
14. (Organizer & Lecturer) June 2016, 2nd Quantum and Computational Chemistry Student Conference (Cass, New Zealand)
    Density-functional theory for molecules
15. (Invited departmental seminar) June 2016, Institute of Fundamental Sciences, Massey University (Palmerston North, New Zealand):
    Density-functional theory using finite and infinite uniform electron gases
16. (Invited departmental seminar) May 2016, Department of Chemistry, University of Canterbury (Christchurch, New Zealand):
    Density-functional theory using finite and infinite uniform electron gases
17. (Invited talk) January 2016, 7th Asia-Pacific Conference of Theoretical and Computational Chemistry (Kaohsiung, Taiwan)
    Three-electron coalescence conditions
18. (Invited talk) September 2014, Molecular Electronic Structure Workshop (Amasya, Turkey):
    How Good are the Hartree-Fock Nodes?
19. (Invited talk) July 2014, Quantum Monte Carlo in the Apuan Alps IX (Vallico Sotto, Italy):
    Electronic-Structure Calculations in a 1D world
20. (Selected talk) July 2014, 14th Theoretical Chemist Meeting (Paris, France):
    DFT and Chemistry in One Dimension
21. (Winter school lecture) June 2014, Quantum and Computational Chemistry Student Conference (Cass, New Zealand):
    Quantum Monte Carlo for electrons

22. (Invited talk) July 2013, Quantum Monte Carlo in the Apuan Alps VIII (Vallico Sotto, Italy):
    Generalized Local Density Approximation in One Dimension

23. (Invited departmental seminar) June 2013, Physics Colloquium, University of Melbourne (Melbourne, Australia):
    Lessons from electron(s) on a (hyper)sphere

24. (Invited talk) June 2011, Mathematical Methods in Quantum Chemistry (Oberwolfach, Germany):
    Lessons from electron(s) on sphere(s)

25. (Departmental seminar) September 2008, COTAW (Namur, Belgium):
    Single-strand breaks induced by low-energy electrons in DNA

26. (Selected talk) July 2008, 10th Theoretical Chemist Meeting (Dinard, France):
    Treatment of biological systems within the Local Self-Consistent Field method

27. (Selected talk) September 2007, 6th Eastern Theoretical Chemist Meeting (Strasbourg, France):
    Theoretical investigation of the geometries and UV/Vis spectra of Poly(L-glutamic acid) featuring photochromic azobenzene side chain.

28. (Departmental seminar) September 2006, Applied Theoretical Chemistry Group (Namur, Belgium):
    Theoretical study of solvent effects on the geometries and the spectroscopic properties of coumarin derivatives.

Poster presentations

1. July 2010, 12th Theoretical Chemist Meeting (Namur, Belgium):
   A tale of two electrons: correlation at high density

2. July 2008, 10th Theoretical Chemist Meeting (Dinard, France):
   Electron attachment on biomolecules: including environment effects with hybrid approaches

3. September 2007, 6th Eastern Theoretical Chemist Meeting (Strasbourg, France):
   Single-strand breaks induced by low-energy electrons in DNA

4. July 2007, Methods and Applications of Computational Chemistry: 2nd Symposium (Kiev, Ukraine):
   QM/MM investigation of single-strand breaks induced by low-energy electrons in DNA

5. November 2006, 15th Conference on Current Trends in Computational Chemistry (Jackson MS, US):
   Self-Consistent Localized Bond Orbitals within the Local Self-Consistent Field Method

6. July 2006, 10th Theoretical Chemist Meeting (Nancy, France):
   Taking the core electrons into account to improve the hybrid Quantum Mechanics/Molecular Mechanics Frontier

7. June 2006, International Society of Quantum Biology and Pharmacology, ISQBP President's Meeting (Strasbourg, France):
   Taking the core electrons into account to improve the hybrid Quantum Mechanics/Molecular Mechanics Frontier

8. June 2005, 5th Eastern Theoretical Chemist Meeting (Reims, France):
   Optimization of localized orbitals within the local Self-Consistent Field method

9. June 2004, 10th Numerical Simulation Workshop (Paris Jussieu, France):
   Structural investigation of polymer-grafted-silica nanoparticles via small-angle neutron scattering: a Monte-Carlo study

Teaching experiences

2017	Teaching assistant Engineering school ISAE-SUPAERO (Toulouse, France) Numerical analysis labs
2016	Senior Lecturer Research School of Chemistry (Australian National University) Third-year course in Computational Chemistry and Molecular Modelling (CHEM3208, course convenor) Honours (fourth-year) course in Theoretical and Computational Chemistry
2006 – 2008	Teaching assistant in Mathematics (64 hours/year during 2 years) Department of Pharmacy (University of Nancy, France) First-year tutorials in Mathematics
2005	Teaching assistant in Physical Chemistry (64 hours) Department of Chemistry (University of Nancy, France) First-year experimental labs
2004	Teaching assistant in Quantum/Computational Chemistry (16 hours) Department of Chemistry (University of Nancy, France) Four-year computational labs