Pierre Mignon

Curriculum Vitae

Maître de Conférences

Equipe physico-Chimie - Institut Lumière Matière
Université Claude Bernard - Lyon1

Thèmes de Recherche abordés

- **Interaction biomolécules/surface** : Etude de l'interaction entre les molécules d'ADN et une surface d'argile hydratée ou pas.
- **Fragmentation de bases d'ADN** : Etude des mécanismes de fragmentation et et comparaisons avec les fragments observé par spectroscopie de masse.
- **Etude de la basicité de Zéolithes** : Adsorption de disproportination de N204 sur la Faujasite Y comportant des cation alcalins.
- **Interactions non-covalentes dans les biomolécules en utilisant les descripteurs DFT de réactivité** : Influence entre liaison hydrogène et le stacking entre les bases d'ADN.

Enseignements

2010– ... **Statistiques**, *2eme Année et Licences Pro.*, IUT Chimie-Lyon1, Cours+TD : 80h/an.

2011– ... **Maîtrise Statistiques des Procédés**, *Licences Pro.*, IUT Chimie-Lyon1, Cours+TD : 10h/an.

2012– ... **Plans d'Expériences**, *2eme Année et Licences Pro.*, IUT Chimie-Lyon1, Cours+TD : 190h/an.

2010–2013 **Méthodes Hartree-Fock et Post-HF**, *Master2*, Réseau Français de Chimie Théorique (Sud-Est), Cours+TD+TP : 14h/an.

2009–2013 **Mathématiques**, *1ere et 2eme Années*, IUT Chimie-Lyon1, Cours+TD : 200h/an.

Post-Docs

2007–2009 **Etude de la polymérisation de l'ADN sur une surface d'argile par des calculs périodiques et dynamique moléculaire**, *Universitat Autonoma Barcelona*, Barcelona Espagne, sous la direction de Prof. M. Sodupe et Prof. P. Ugliengo.

2005–2007 **Etude théorique des zéolithes basiques par les descripteurs de réactivités issus de la DFT et calculs périodiques**, *Katholieke Universiteit Leuven - Centre pour la Chimie de Surface et la Catalyse*, Leuven Belgique, sous la direction de Prof. R. Schoonheydt.

bâtiment Kastler - 43 bd du 11 novembre 1918
69622 Villeurbanne Cedex, France
☎ *[+33](0)4 72 44 83 14* • ✉ *pierre.mignon@univ-lyon1.fr*

Doctorat

2001–2005 **Etude Théorique de l'Influence entre Interactions Non-covalentes dans les Biomolecules**

Département de Chimie Générale Chemistry, Vrije Universiteit Brussel, Bruxelles

Directeurs : Prof. P. Geerlings, Chimie Générale & Prof. J. Steyaert, Ultra-structure

Formation

1999–2000 **DEA de chimie Informatique et Théorique**, *Université Henry Poincaré*, Nancy.
Stage (6 mois) : *Etude de la catalyse de l'ozonolyse d'alcène par l'oxyde de Magnésium. Elaboration d'une méthode de calcul des intégrales de Roothaan en condition asymptotique*, sous la direction de Prof. F. Hoggan

1998–1999 **Maîtrise en Sciences Physiques**, *Université Blaise Pascal*, Clermont-Ferrand.
Stage (3 mois) : *Etude de la Chimisorption de la biocytin sur une électrode de carbone en utilisant des méthodes semi-empiriques*, sous la direction de Prof. F. Hoggan

Production Scientifique

Publications

2015 29. *Fragmentation Mechanisms of Cytosine, Adenine and Guanine Ionized Bases*, L. S. Arani, P. Mignon, H. Abdoul-Carime, B. Farizon, B M. Farizon, H. Chermette, **Phys. Chem. Chem. Phys.**, *soumis*

2014 28. *Dual Descriptor and Molecular Electrostatic Potential : Complementary Tools for the Study of the Coordination chemistry of Ambiphilic Ligands*, F. Guegan, P. Mignon, V. Tognetti, L. Joubert, C. Morell, **Phys. Chem. Chem. Phys.**, 2014, 16, 15558-15569

27. *Theoretical and experimental study of the fragmentation of protonated uracil*, L. Sadr-Arani, P. Mignon, H. Chermette, T. Douki, **Chem. Phys. Let.**, 2014, 605-606, 108-114.

26. *Mechanism of addition-fragmentation reaction of thiocarbonyls compounds in free radical polymerization. A DFT study*, N. Latelli, N. Ouddai, M. Arotçaréna, P. Chaumont, P. Mignon, H. Chermette, **Comp. Theor. Chem.**, 2014, 1027, 39-45.

2013 25. *Structural Behaviors of Cytosine into the Hydrated Interlayer of Na+ Montmorillonite Clay. An ab-initio Molecular Dynamics Study.*, P. Mignon, M. Sodupe, **J. Phys. Chem. C.**, 2013, 117, 26179–26189.

24. *Assessing the performances of some recently proposed density functionals for the description of organometallic structures*, E. Bremond, M. Poor Kalhor, D. Bousquet, P. Mignon, I. Ciofini, C. Adamo, P. Cortona, H. Chermette, **Theor. Chem. Acc.**, 2013, 132, 1401-1412.

23. *Quantitative structure-activity relationship to predict acute fish toxicity of organic solvents*, A Levet, C Bordes, Y Clément, P. Mignon, H Chermette, P Marote, C Cren-Olivé, P Lantéri, **Chemosphere**, 2013, 93, 1094-1103.

22. *Hydrogen release from charged fragments of the uracil cation followed by their fragmentation : A DFT study*, L. S. Arani, P. Mignon, H. Abdoul-Carime, B. Farizon, B M. Farizon, H. Chermette, **Chem. Phys. Lett.**, 2013, 583, 165-169.

21. *Unusual Reactivities of Acridine Derivatives in Catalytic Hydrogenation. A Combined Experimental and Theoretical Study*, P. Mignon, M. Tiano, P. Belmont, A. Favre-Réguillon, H. Chermette , F. Fache, **J. Mol. Cat. A : Chemical**, 2013, 371, 63-69.

2012 20. *Cooperative effects at water-crystalline silica interfaces strengthen surface silanol hydrogen bonding. An ab initio molecular dynamics study*, F. Musso, P. Mignon, P. Ugliengo, M. Sodupe, **Phys. Chem. Chem. Phys.**, 2012, 14, 10507-10514.

19. *DFT study of the fragmentation mechanism of uracil RNA base*, L. S. Arani, P. Mignon, H. Abdoul-Carime, B. Farizon, B M. Farizon, H. Chermette, **Phys. Chem. Chem. Phys.**, 2012, 14, 9855-9870.

18. *Study of Prepolymerization Complex Formation in the Synthesis of Steroid-Based Molecularly Imprinted Polymers*, C. Sanglar, T. Jansen, M. C. Silaghi, J. Mernier, P. Mignon, H. Chermette, **Analytical Chem.**, 2012, 84, 4481-4488.

17. *Theoretical study of the adsorption of DNA bases on the acidic external surface of montmorillonite*, P. Mignon, M. Sodupe, **Phys. Chem. Chem. Phys.**, 2012, 14, 945-954.

16. *Oxo iron(IV) as an oxidative active intermediate of p-chlorophenol in the Fenton reaction : a DFT study*, P. Mignon, M. Pera-Titus, H. Chermette, , 2012, 14, 3766-3774.

15. *Theoretical study of the polymerization of p-tert-butyl-anisol*, S. Ayadi, P. Mignon, M. Abderrabba, H. Chermette, **Int. J. Quantum Chem.**, 2012, 112, 2154-2159.

2010 14. *Ab initio molecular dynamics study of the hydration of Li+, Na+ and K+ in a Montmorillonite model. Influence of isomorphic substitution*, P. Mignon, P. Ugliengo, M. Sodupe and E. R. Hernandez, **Phys. Chem. Chem. Phys.**, 2010, 12, 688-697.

2009 13. *Theoretical Study of the Adsorption of RNA/DNA Bases on the External Surfaces of Na+Montmorillonite*, P. Mignon, P. Ugliengo and M. Sodupe, **J. Phys. Chem. C.**, 2009, 113, 13741–13749.

2008 12. *Understand the Reactivity and Basicity of Zeolites. A periodic DFT study of the N2O4 Disproportionation over Alkaline Cation Exchanged zeolite Y*, P. Mignon, E. A. Pidko, R. A. van Santen, P. Geerlings and R. A. Schoonheydt, **Chemistry. Eur. J.**, 2008, 14, 5168-5177.

11. *Molecular recognition of N2O4 on alkali-exchanged zeolites X. A periodic density functional theory study*, E. A. Pidko, P. Mignon, P. Geerlings, R. A. Schoonheydt and R. A. van Santen, **J. Phys. Chem. C.**, 2008, 112, 5510-5519.

2007 10. *Oxygen Basicity in Alkaline Cation-Exchanged Zeolite and the Effect of Isomorphous Substitution. Use of Hard Descriptors*, P. Mignon, P. Geerlings, R. Schoonheydt, **J. Phys. Chem. C.**, 2007, 111 ; 12376-12382.

2006 9. *Understanding the Concept of Basicity in Zeolites : a DFT study*, P. Mignon, P. Geerlings, R. Schoonheydt, **J. Phys. Chem. B.**, 2006, 110, 24947-24954.

8. *Influence of Stacking on the Hydrogen Bond Donating Potential of Nucleic Bases*, Vanommeslaeghe, K., Mignon, P., Loverix, S., Tourwe, D., Geerlings, P., **J. Chem. Theory and Comput.**, 2006, 2, 1444-1452.

7. *Probing the Basicity of Zeolite frameworks with N2O4 : a DFT approach*, A.M. Vos, P. Mignon, P. Geerlings, F. Thybault-Starzyk and R.A. Schoonheydt, **Microporous and Mesoporous Materials**, 2006, 90, 370-376.

2005 6. *The Effect of Stacking Interaction on the pKa of Phenol stacked with Substituted Benzenes*, O. Andrasz, P. Mignon, F. De Proft, T. Veszprémi, P. Geerlings, **Chem. Phys. Letters**, 2005, 407, 504-509.

5. *Influence of the π-π Interaction on the Hydrogen Bonding Capacity of Stacked DNA/RNA Bases*, P. Mignon, S. Loverix, J. Steyaert, P. Geerlings, **Nucleic Acids Research**, 2005, 33, 1779-1789.

4. *Interplay between π-π interactions and the H-bonding ability of aromatic nitrogen bases*, P. Mignon, S. Loverix, P. Geerlings, **Chem. Phys. Letters**, 2005, 401, 40-46.

2004 3. *Influence of Stacking on Hydrogen Bonding : Quantum Chemical Study on Pyridine-Benzene Model Complexes*, P. Mignon, S. Loverix, J. Steyaert, P. Geerlings, **J. Phys. Chem. A**, 2004, 108, 6038-6044.

2. *Functional Assessment of "In Vivo" and "In Silico" Mutations in the Guanine Binding Site of RNase T1 : A DFT Study*, P. Mignon, S. Loverix, F. De Proft, P. Geerlings, **Int. J. Quantum Chem.** , 2004, 99, 53-58.

2002 1. *A Nucleophile Activation Dyad in Ribonucleases. A Combined X-RAY Crystallographic/ab Initio Quantum Chemical Study*, P. Mignon, J. Steyaert, R. Loris, P. Geerlings, S. Loverix., **J. Biol. Chem.**, 2002, 277, 36770–36774.

Présentations Orales et Séminaires

2015 7. *Hydrated Montmorillonite interlayer properties and adsorption of DNA nucleobases studied through static and MD ab-initio simulations.*, P. Mignon, M. Sodupe, **CECAM Workshop - Atomistic Simulations in Earth Sciences**, Paris, France, 18 Juin 2015

2014 6. *Structural Behaviors of Cytosine into the Hydrated Interlayer of Na+ Montmorillonite Clay. An ab-initio Molecular Dynamics Study.*, P. Mignon, M. Sodupe, **CECAM Workshop - Simulation of Biomolecular Interactions with Inorganic and Organic Surfaces as a Challenge for Future Nanotechnologies**, Toulouse, France, 26 Mars 2014

2007 5. *Theoretical Studies of The Intherplay between Non Covalent Interactions in Biomolecules*, Mignon P., Steyaert J., Loverix S., Geerlings P., **Scientific Research Network - Bio-Applications Of Density Functional Theory Quantum Chemistry : Fundamental and Applied Aspects of Density Functional Theory**, Ghent, Belgique, 24 Mai 2007

2006 4. *The Influence of Aromatic Stacking on the H-Bonding Capacity in Biomolecules*, Mignon P., Steyaert J., Loverix S., Geerlings P., **Chemical reactivity Congress, Theoretical Aspects of Reactivity**, Vrije Universiteit Brussel, Bruxelles, Belgique, 7 Avril 2006

3. *Basicity of Zeolite*, Mignon P., Vos A., Geerlings P., Schoonheydt R., **Netherlands' Catalysis and Chemistry Conference VII**, Noordwijkerhout, Pays-Bas, 8 Mars 2006

2. *Lewis Acidity vs. Oxygen Basicity in Cation Exchanged Zeolites. A DFT Study of the Methylation of Al-O-Si Bridging Oxygen*, Mignon P., Geerlings P., Schoonheydt R., **Lewis acidity in Catalysis workshop**, Leuven, Belgique, 7 Décembre 2006

2002 1. *Nucleophile activation in Ribonucleases*, Mignon P., Steyaert J., Loverix S., Geerlings P., **6de Vlaams Jongerencongres van de chemie**, Universiteit Antwerpen UIA, Belgium, 9 Avril 2002

Présentations par Affiche

2014 15. *Ab-initio MD simulation of the interaction between DNA nucleobases and clay hydrated interlayer*, P. Mignon, M. Sodupe, **Next generation quantum based molecular dynamics : challenges and perspectives**, Bremen, Allemagne, 13-17 Juillet 2015

2012 15. *DFT Study of the Fragmentation of Uracil*, L. S. Arani, P. Mignon, H. Abdoul-Carime, B. Farizon, B M. Farizon, H. Chermette, **Challenges in Density Matrix and Density Functional Theory**, Ghent, Belgique, 1-6 Avril 2012

2011 14. *Adsorption of Nucleobases on Montmorillonite Clay*, Mignon P., Ugliengo P., Sodupe M., **WATOC2011 : Theoretical modeling of materials**, Barcelona, Espagne, 13-15 Juillet 2011

2009 13. *Ab Initio Molecular Dynamics Study of the Hydration of Li+, Na+ and K+ Montmorillonite*, Mignon P., Ugliengo P., Sodupe M., Hernandez E., **DFT2009**, Lyon, France, 31 Aout 4 Septembre 2009

2008 12. *Theoretical Study of the Adsorption of RNA bases on a Surface of Na+-Montmorillonite*, Mignon P., Ugliengo P., Sodupe M., **ISSOL Meeting : XV international Conference on the Origin of Life**, Florence, Italy, 24-29 Aout 2008

2007 11. *Site Identification of the N2O4 Disproportionation in Faujasite Y. A Periodic DFT Study*, Mignon P., E. A. Pidko, R. A. van Santen, P. Geerlings, R. A. Schoonheydt, **DFT2007**, Amsterdam, Pays-Bas, 26-30 Aout 2007

2006 10. *Probing the Basicity of Alkali-metal exchanged Zeolites using Isomorphous Substitution. A DFT Study*, Mignon P., Geerlings P., Schoonheydt R., **ICTAC-11 : 11th International Conference on Theoretical Aspects of Catalysis**, Berlin, Allemagne, 11-14 Juin 2006

9. *A Density Functional Theory Study on the Basicity of Alkali Cation-Exchanged Zeolites*, Mignon P. Geerlings P., Schoonheydt R., **Chemical Reactivity Congress, Theoretical Aspects of Reactivity**, Vrije Universiteit Brussel, Bruxelles, Belgique, April 7 Avril 2006

2005 8. *Role of Local and Global DFT based indices in the Estimation of Interaction Energy Components in Stacked Complexes*, Mignon P., Loverix P., Steyaert J., Geerlings P, **DFT2005**, Genève, Suisse, 11-15 Septembre 2005

7. *Influence of the Electrostatic Interaction between Stacked RNA-DNA Bases on their H-Bonding Capacity*, Geerlings P., Mignon P., Loverix S., Steyaert J., De Proft F., **WATOC 2005, Modeling Structure and Reactivity**, Cape Town, Afrique du Sud, 16-21 Janvier 2005

2004 6. *Effect of stacking upon the hydrogen bonding capacity of an aromatic nitrogen. The use of DFT based reactivity indices in the prediction of the stacking interaction*, Mignon P., Loverix S., Geerlings P., **Molecules of Biological Interest in the Gas Phase**, Exeter, UK,13-18 Avril 2004

2003 5. *Guanine binding in RNase T1 : a DFT study*, Mignon P., Steyaert J., Loverix S., Geerlings P., **DFT2003 : 10th International Conference on the Applications of Density Functional Theory in Chemistry and Physics**, Vrije Universiteit Brussels, Bruxelles, Belgique 7-12 Septembre 2003

4. *A catalytic dyad for nucleophile activation in Ribonucleases*, Mignon P., Steyaert J., Loverix S., Geerlings P., **Modelling chemical reactivity : from gas-phase to solution and enzymes**, Nancy, France, 16-18 Juillet 2003

2002 3. *Quantum chemical study on the binding and catalytic properties of RNase T1*, Mignon P., Steyaert J., Loverix S., Geerlings P., **Molecules of Biological Interest in the Gas Phase**, Wildbad Kreuth, Allemagne, 21-26 Juiller 2002

2. *A nucleophile activation dyad in ribonucleases. A combined X-Ray crystallographic / ab-initio quantum chemical approach*, Mignon P., Steyaert J., Loverix S., Geerlings P., **6th International meeting on Ribonucleases**, Bath, UK, 19-23 Juin 2002

2001 1. *Quantum chemical study on the influence of mutations on binding and catalysis of RNase T1*, Mignon P., Steyaert J., Loverix S., Geerlings P., **7eme universite d'été de Phisico-Chimie Theorique**, Aussois, France, September 30 Septembre-5 Octobre 2001