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Date of birth 16th February 1984
Nationality French
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Assistant Professor at the Laboratory of Quantum Chemistry and Quantum Physics

RESEARCH EXPERIENCE

2020 **Habilitation to Supervise Researches** (March 2020, Université Paul Sabatier): Theoretical study of the physicochemical properties of aqueous systems: from the gas to the condensed phase.

2016 - 2018 Two half-years **CNRS delegation** at LCPQ.

2012 - *now* **Assistant Professor** in the Laboratoire de Chimie et Physique Quantiques (LCPQ), UMR CNRS 5626, at the University Paul Sabatier.

2010 - 2012 **Post-Doct** in the Department of Chemistry and Applied Biosciences of the ETH Zürich and in the Facoltà di Informatica, Istituto di Scienze Computazionali, at the Università della Svizzera Italiana, in the group Pr. M. Parrinello.

2007 - 2010 **PhD** at the Ecole Nationale Supérieure de Chimie de Rennes under the supervision of Pr. R. Gautier in the «Sciences Chimiques de Rennes» Laboratory, UMR CNRS 6226, France
«Solid-State NMR and modeling: converging tools for the development of new materials»

TRAINING ET DIPLOMA

2007 - 2010 **PhD in Chemistry at the Ecole Nationale Supérieure de Chimie de Rennes** (with distinction) under the supervision of Pr. R. Gautier in the «Sciences Chimiques de Rennes» Laboratory, UMR CNRS 6226, France
PhD defended the 24th of September 2010 at the ENSCR in front of the jury composed by D. Massiot, R. Poteau, J.-F. Halet, L. Delevoye, L. Le Pollès, R. Gautier, P. Gougeon and C. J. Pickard
«Solid-State NMR and modeling: converging tools for the development of new materials»

2007 **Master of Solid-State and Material Chemistry** from the University of Rennes 1 option Theoretical Chemistry (upper second class honors)
Engineering diploma of the Ecole Nationale Supérieure de Chimie de Rennes

2006 **Training period** at the **McMaster University** (Ontario, Canada) (4 months)
Subject: «Inner-shell excitation of gas phase carbonates and α,γ-dicarbonyl compounds»
Supervisor: Pr. A. P. Hitchcock

2004 - 2007 **Chemistry Engineering Student** at the Ecole Nationale Supérieure de Chimie de Rennes (France). Diploma obtained in 2007.

SCIENTIFIC PUBLICATIONS

1. *Inner-Shell Excitation of Gas Phase Carbonates and α,γ-dicarbonyl Compounds*
   R. Lessard, **J. Cuny**, G. Cooper, A. P. Hitchcock
   Chem. Phys. **2007**, *331*, 289-303

2. *DFT Calculations of Quadrupolar Solid-State NMR Properties. Some Examples in Solid-State Inorganic Chemistry*
   J. Cuny, S. Messaoudi, V. Alonzo, E. Furet, J.-F. Halet, E. Le Fur, S. E. Ashbrook, C. J. Pickard, R. Gautier, L. Le Pollès
   J. Comput. Chem. **2008**, *29*, 2279-2287

3. *Redetermination of $Zn_2Mo_3O_8$*
   J. Cuny, P. Gougeon, P. Gall
   Acta Cryst. **2009**, *E65*, i51

4. *Synthesis, Electronic and Crystal Structures, and Physical Studies of the Superconductor $Cs_{\sim 1}Mo_{12}S_{14}$, Final Step of the Condensation of the $Mo_6L_8^iL_6^a$ Unit*
   P. Gougeon, D. Salloum, **J. Cuny**, L. Le Pollès, M. Le Floch, R. Gautier, M. Potel
   Inorg. Chem. **2009**, *48*, 8337-8341

5. *Density Functional Theory Calculations of ^{95}Mo NMR Parameters in Solid-State Compounds*
   J. Cuny, E. Furet, R. Gautier, L. Le Pollès, C. J. Pickard, J.-B. d'Espinose de Lacaillerie
   ChemPhysChem. **2009**, *10*, 3320-3329

6. *Improving Sensitivity and Resolution of MQMAS Spectra: A ^{45}Sc Case Study of Scandium Sulphate Pentahydrate*
   C. V. Chandran, **J. Cuny**, R. Gautier, L. Le Pollès, C. J. Pickard, T. Bräuniger
   J. Magn. Reson. **2010**, *203*, 226-235

7. *Electric Field Gradient Calculations in Paramagnetic Compounds Using the PAW Approach. Application to ^{23}Na NMR in Layered Vanadium Phosphates*
   J. Cuny, J. R. Yates, R. Gautier, E. Furet, E. Le Fur, L. Le Pollès
   Magn. Reson. Chem. **2010**, *48*, S171-S175

8. *High-Temperature Experimental and Theoretical Study of Magnetic Interactions in Diamond and Pseudo-Diamond Frameworks Built up from Hexanuclear Tantalum Clusters*
   B. Peric, S. Cordier, **J. Cuny**, R. Gautier, T. Guizouarn, P. Planinic
   Chem.--Eur. J. **2011**, *17*, 6263

9. *^{95}Mo nuclear magnetic resonance parameters of molybdenum hexacarbonyl from density functional theory: appraisal of computational and geometrical parameters*
   J. Cuny, K. Sykina, B. Fontaine, L. Le Pollès, C. J. Pickard, R. Gautier
   Phys. Chem. Chem. Phys. **2011**, *13*, 19471-19479

10. *Exploring the free energy surfaces of clusters using reconnaissance metadynamics*
    G. A. Tribello, **J. Cuny**, H. Eshet, M. Parrinello
    J. Chem. Phys. **2011**, *135*, 114109

11. *Synthesis, Crystal and Electronic Structures, and Magnetic Properties of the $LiLn_9Mo_{16}O_{35}$ (Ln = La, Ce, Pr, and Nd) Compounds Containing the Original Cluster $Mo_{16}O_{36}$*
    P. Gougeon, P. Gall, **J. Cuny**, R. Gautier, L. Le Pollès, L. Delevoye, J. Trébosc
    Chem.--Eur. J. **2011**, *17*, 13806–13813

12. *The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates*
    A. A. Hassanali, **J. Cuny**, M. Ceriotti, C. J. Pickard, M. Parrinello
    J. Am. Chem. Soc. **2012***, 134,* 8557-8569

13. *^{95}Mo Solid-State Nuclear Magnetic Resonance Spectroscopy and Quantum Simulations : Synergetic Tools for the Study of Molybdenum Cluster Materials*
    J. Cuny, S. Cordier, C. Perrin, C. J. Pickard, L. Delevoye, J. Trèbosc, Z. Gan, L. Le Pollès, R. Gautier
    Inorg. Chem. **2013**, *52*, 617-627

14. *Synthesis, crystal and electronic structures and magnetic properties of $Li_2SnMo_3O_8$:A novel reduced molybdenum oxide containing Mo_3O_{13} cluster units*
    P. Gall, R. Al Rahal Al Orabi, T. Guizouarn, **J. Cuny**, B. Fontaine, R. Gautier, P. Gougeon
    J. Solid State Chem. **2013**, *201*, 312-316

15. *Shape Modulation of Octanuclear Cu(I) or Ag(I) Dichalcogeno Template Clusters with Respect to the Nature of their Encapsulated Anions: A Combined Theoretical and Experimental Investigation*
    C. Latouche, S. Kahlal, E. Furet, P.-K. Liao, Y.-R. Lin, C.-S. Fang, **J. Cuny**, C. W. Liu, J.-Y. Saillard
    Inorg. Chem. **2013**, *52*, 617-627

16. *Proton transfer through the water gossamer*
    A. A. Hassanali, F. Giberti, **J. Cuny**, T. D. Kühne, M. Parrinello
    PNAS **2013**, *110*, 13723-13728

17. *Nuclear quantum effects and hydrogen bond fluctuations in water*

M. Ceriotti, **J. Cuny**, M. Parrinello, D. E. Manolopoulos
PNAS **2013**, *110*, 15591-15596

18. *Aqueous solutions: state of the art in ab initio molecular dynamics*
A. A. Hassanali, **J. Cuny**, V. Verdolino, M. Parrinello
Phil. Trans. R. Soc. A **2014**, *372*, 20120482

19. *Ab Initio Molecular Dynamics Study of the Mechanism of Proton Recombination with a Weak Base*
J. Cuny, A. A. Hassanali
J. Phys. Chem. B **2014**, *118,* 13903-13912

20. *Phase changes of the water hexamer and octamer in the gas phase and adsorbed on polycyclic aromatic hydrocarbons*
L. F. L. Oliveira, **J. Cuny**, M. Morinière, L. Dontot, A. Simon, F. Spiegelman, M. Rapacioli
Phys. Chem. Chem. Phys. **2015**, *17*, 17079-17089

21. *Evaluation of ^{95}Mo Nuclear Shielding and Chemical Shift of $[Mo_6X_{14}]^{2-}$ Clusters in the Liquid Phase*
T. T. Nguyen, J. Jung, X. Trivelli, J. Trébosc, S. Cordier, Y. Molard, L. LePollès, C. J. Pickard, **J. Cuny**, R. Gautier
I*norg. Chem.* **2015**, *54*, 7673-7683

22. *Combined theoretical and time-resolved photoluminescence investigations of $[Mo_6Br^i_8Br^a_6]^{2-}$ metal cluster units: evidences of dual emission*
K. Costuas, A. Garreau, A. Bulou, B. Fontaine, **J. Cuny**, R. Gautier, M. Mortier, Y. Molard, J.-L. Duvail, E. Faulques, S. Cordier
Phys. Chem. Chem. Phys. **2015**, *17*, 28574

23. *Cationic Methylene-Pyrene Isomers and Isomerization Pathways: Finite Temperature Theoretical Studies*
M. Rapacioli, A. Simon, C. Marshall, **J. Cuny**, D. Kokkin, F. Spiegelman, C. Joblin
J. Phys. Chem. A **2015**, *119*, 12845-12854

24. *Ab-initio Quality NMR Parameters in Solid-State Materials using a High-Dimensional Neural-Network Representation*
J. Cuny, Y. Xie, C. J. Pickard, A. A. Hassanali
J. Chem. Theory Comput. **2016**, *12* (2), 765-773

25. *Benchmarking DFTB for Silver and Gold Materials: From Small Clusters to Bulk*
L. F. L. Oliveira, N. Tarrat, **J. Cuny**, J. Morillo, D. Lemoine, F. Spiegelman, M. Rapacioli
J. Phys. Chem. A **2016**, *120*, 8469-8483

26. *Structural Characterisation of Sulfur-Containing Water Clusters Using a Density-Functional Based Tight-Binding Approach*
K. A. Korchagina, A. Simon, M. Rapacioli, F. Spiegelman, **J. Cuny**
J. Phys. Chem. A **2016**, *120*, 9089-9100

27. *Keto-polymethines: a versatile class of dyes with outstanding spectroscopic properties for in cellulo and in vivo two-photon microscopy imaging*
S. Pascal, S. Denis-Quanquin, F. Appaix, A. Duperray, A. Grichine, B. Le Guennic, D. Jacquemin, **J. Cuny**, S.-H. Chi, J. W. Perry, B. van der Sanden, C. Monnereau, C. Andraud, O. Maury
Chem. Sci. **2017,** *8*, 381-394

28. *Metadynamics combined with Auxiliary Density Functional and Density Functional Tight Binding Methods: Alanine Dipeptide as a Case Study*
J. Cuny, K. Korchagina, C. Menakbi T. Mineva
J. Mol. Model., **2017**, *23*, 71

29. *Global Optimization of Neutral and Charged 20- and 55-Atom Silver and Gold Clusters at the DFTB Level*
N. Tarrat, M. Rapacioli, **J. Cuny**, J. Morillo, F. Spiegelman
Comp. Theor. Chem., **2017**, *1107*, 102-114

30. *Pesticide interaction with environmentally important cations: A molecular dynamics and DFT study of metamitron and fenhexamid*
B. Belzunces, S. Hoyau, **J Cuny**, F. Bessac
Comp. Theor. Chem., **2017**, *1117*, 220-234.

31. *Theoretical Investigation of the Solid-Liquid Phase Transition in Protonated Water Clusters*
K. Korchagina, A. Simon, M. Rapacioli, F. Spiegelman, J.-M. L'Hermite, I Braud, S. Zamith, **J. Cuny**
PCCP, **2017**, *19*, 27288-27298.

32. *Molecular Dynamics Study of the Collision-Induced Reaction of H with CO on Small Water Clusters*
K. Korchagina, F. Spiegelman, **J. Cuny**
J. Phys. Chem. A, **2017**, *121*, 9485-9494.

33. *Conformational Study and Chiroptical Properties of Chiral Dimethyl- Ethylenedithio-Tetrathiafulvalene (DM-EDT-TTF)*
T. Cauchy, F. Pop, **J. Cuny**, N. Avarvari
Chimia, **2018**, *72*, 1-5.

34. *Density-functional tight-binding approach for metal clusters, nanoparticles, surfaces and bulk: application to silver and gold*
J. Cuny, N. Tarrat, F. Spiegelman, A. Huguenot, A. Rapacioli
J. Phys.: Condens. Matter, **2018**, *30*, 30.

35. *Metal Atom Clusters as Building Blocks for Multifunctional Proton-Conducting Materials: Theoretical and Experimental Characterization*
G. Daigre, **J. Cuny**, P. Lemoine, M. Amela-Cortes, S. Paofai, N. Audebrand, A. Le Gal La Salle, E. Quarez, O. Joubert, N. G. Naumov, S. Cordier
Inorg. Chem., **2018**, *57,* 9814–9825.

36. *Evaluation of Gas-to-Liquid ^{17}O Chemical Shift of Water: A Test Case for Molecular and Periodic Approaches*
J. Cuny, F. Jolibois, I. C. Gerber
J. Chem. Theory Comput., **2018**, *14,* 4041-4051

37. *Selective assembly of Molybdenum Clusters into Nanomarbles and Nanocapsules*
F. Sciortino, **J. Cuny**, F. Grasset, C. Lagrost, P. Lemoine, A. Moréac, Y. Molard, T. Takei, S. Cordier, S. Chevance , F. Gauffre
ChemComm, **2018***, 54,* 13387-13390.

38. *Contribution of the Density-Functional based Tight-Binding Scheme to the Description of Water Clusters : Methods, Applications and Extension to Bulk Systems*
A. Simon, M. Rapacioli, E. Michoulier, L. Zheng, K. Korchagina, **J. Cuny**
Mol. Sim., **2019***, 45,* 249-268

39. *Size-Dependent Proton Localization in Hydrated Uracil Clusters: A Joint Experimental and Theoretical Study*
I. Braud, S. Zamith, **J. Cuny**, L. Zheng, J.-M. L'Hermite
J. Chem. Phys., **2019***, 150*, 014303

40. *Molecular Simulations with in-deMon2k QM/MM, a Tutorial-Review*
A. de la Lande, A. Alvarez-Ibarra, K. Hasnaoui, F. Cailliez, X. Wu, T. Mineva, **J. Cuny**, P. Calaminici, L. López-Sosa, G. Geudtner, I. Navizet, C. G. Iriepa, D. R. Salahub, A. M. Köster
Molecules, **2019**, *24*, 1653

41. *Density-functional tight-binding: basic concepts and applications to molecules and clusters*
F. Spiegelman, N. Tarrat, J Cuny, L. Dontot, E. Posenitskiy, C. Marti, A. Simon, M. Rapacioli
Advances in Physics: X, **2020***, 5(1)*, 1710252.

BOOK CHAPTERS

1. *First-Principles Computation of NMR Parameters in Solid-State Chemistry*
J. Cuny, R. Gautier, J.-F. Halet
Handbook of Solid State Chemistry, Volume 5 - Theoretical Description, **2017**, Wiley-VCH

POSTER COMMUNICATIONS

1. *Electronic Structure Analysis of New Molybdenum Oxide Cluster Compounds*
J. Cuny, L. Le Pollès, P. Gall, R. Gautier, P. Gougeon
International Workshop on Transition Metal Clusters, Rennes (France), July 2008

2. *Combined High Field ^{95}Mo Solid State NMR and DFT Calculated Electric Field Gradients as a Tool for Cluster Science*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye
International Workshop on Transition Metal Clusters, Rennes (France), July 2008

3. *Calculs DFT de paramètres de RMN du ^{95}Mo par une approche périodique*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye, J. B. d'Espinose de Lacaillerie
11ème Rencontre des Chimistes Théoriciens Francophones, Dinard (France), July 2008

4. *Validation of Projector Augmented-Wave Methods for the Calculation of NMR Properties of Molybdenum*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye, J. B. d'Espinose de Lacaillerie
14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste (Italy), January 2009

5. *^{95}Mo Solid-State NMR Study of Transition Metal Cluster Compounds: A Synergic Experimental and Computational Approach*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye
EUROMAR 2009, Göteborg (Sweden), July 2009

6. *Validation of Projector Augmented-Wave Methods for the Calculation of NMR Properties of Molybdenum*
J. Cuny, K. Sykina, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye
13th International Conference on the Application of Density Functional Theory in Chemistry and Physics. DFT09, Lyon (France), September 2009

7. *Evidence and Characterisation of Nuclear Quantum Effects in Condensed Matter*
J. Cuny, A. A. Hassanali, M. Ceriotti, M. Deschamps, M. Parrinello
CPMD 2013, Leipzig (Germany), September 2013

8. *Evidence and Characterisation of Nuclear Quantum Effects in Condensed Matter*
J. Cuny, A. A. Hassanali, M. Ceriotti, M. Deschamps, M. Parrinello
ICAMM 2014, Nantes (France), July 2014

9. *Application de l'approche SCC-DFTB pour l'étude des interactions CO-X (X=H_2O, H^+, H_3O^+)*
K. Korchagina, J. Cuny, A. Simon, M. Rapacioli, F. Spiegelman
14ème Rencontre des Chimistes Théoriciens Francophones, Paris (France), July 2014

10. *Molecular dynamics study of the H and CO recombination on small water clusters*
K. Korchagina, J. Cuny, A. Simon, M. Rapacioli, F. Spiegelman
Molecular Dynamics Summer School: The Computer Simulation of Condensed Phases "CCP5", Manchester (Royaume-Uni), July 2015

11. *Influence de la nature d'espèces sulfurées sur les propriétés physico-chimiques de clusters de molécules d'eau*
K. Korchagina, J. Cuny, A. Simon, M. Rapacioli, F. Spiegelman
15ème Rencontre des Chimistes Théoriciens Francophones, Lyon (France), July 2016

12. *New functionalities of deMon2k for user-friendly QM/MM simulations*
A. de la Lande, T. Mineva, **J. Cuny**
deMon Workshop 2019, Frejus (France), May 2019

13. *Synchronous and Asynchronous implementation of the Parallel-Tempering Molecular Dynamics method in the codes deMonNano and deMon2k*
F. Louisnard, A. Simon, J. Cuny
TOUCAM 2019, Toulouse (France), November 7-8 2019

ORAL COMMUNICATIONS

1. *Calculs DFT de paramètres de RMN du ^{95}Mo par une approche périodique*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye
Journée de travail du réseau RMN structurale dans le Grand Bassin Parisien, Rennes (France), June 2008

2. *DFT Investigations of the Structural and Physical Properties of New Solid-State Transition Metal Cluster Compounds*
J. Cuny, B. Fontaine, S. Cordier, **R. Gautier**, P. Gougeon, J.-F. Halet, L. Le Pollès, C. Perrin, C. J. Pickard
International Symposium on Structure-Property Relationships in Solid State Materials, Nantes (France), July 2008

3. *Solid-state NMR and DFT calculations: A Combined Tool for the Study of Transition Metal Compounds*
J. Cuny, L. Le Pollès, **R. Gautier**, C. J. Pickard, J. Trebosc, L. Delevoye
16th International Conference on Solid Compounds of transition Elements, Dresden (Germany), July 2008

4. *RMN du solide et modélisation : outils convergents pour le développement de nouveaux matériaux*
J. Cuny, R. Gautier, L. Le Pollès, C. J. Pickard, J. Trebosc, L. Delevoye
Journées Scientifiques de la Société Chimique de France Section Bretagne - Pays de la Loire, Trégastel (France), May 2009

5. *Etude de composés à clusters de molybdène par une approche combinée calculs quantiques et RMN ^{95}Mo en phase solide*
J. Cuny, R. Gautier, L. Le Pollès, C. J. Pickard, J. Trebosc, L. Delevoye
Journée de travail du réseau RMN structurale dans le Grand Bassin Parisien, Caen (France), June 2009

6. *Solid State NMR and DFT Calculations: A Combined Tool for the Study of Transition Metal Materials*
J. Cuny, L. Le Pollès, **R. Gautier**, C. J. Pickard, L. Delevoye, J. Trebosc
6ème rencontre franco-espagnole sur le chimie et la physique de l'état solide, Tarragona (Spain), March 2010

7. *RMN du solide et modélisation : outils convergents pour le développement de nouveaux matériaux*
   J. Cuny, R. Gautier, L. Le Pollès, C. J. Pickard, J. Trebosc, L. Delevoye
   Journée des doctorants de l'UMR 6226, Université Rennes 1, Rennes (France), Mai 2010

8. *Apport du calcul quantique à l'étude RMN du solide de composés inorganiques de l'état solide*
   J. Cuny, R. Gautier, L. Le Pollès, C. J. Pickard
   12ème Rencontre des Chimistes Théoriciens Francophones, FUNDP, Namur (Belgium), July 2010

9. *^{95}Mo Solid-State NMR Study of Transition Metal Cluster Compounds: A Synergetic Experimental and Computational Approach*
   J. Cuny, R. Gautier, L. Le Pollès, J. Trebosc, L. Delevoye, C. J. Pickard,
   52nd Rocky Mountain Conference on analytical Chemistry, Snowmass Colorado (USA), August 2010

10. *Transition Metal Cluster Compounds Studied by a Combined ^{95}Mo Solid-State NMR and DFT Approach*
    J. Cuny, B. Fontaine, S. Cordier, P. Gall, **R. Gautier**, P. Gougeon, J.-F. Halet, L. Le Pollès, Y. Molard, C. Perrin, M. Potel, C. J. Pickard
    2nd International Workshop on Transition Metal Clusters, Rostock (Germany), September 2010

11. *Calcul quantique et réseau de neurones, nouvelle approche pour l'étude RMN en température de systèmes amorphes complexes*
    J. Cuny, Y. Xue, A. A. Hassanali, C. J. Pickard, M. Parrinello
    Journée de travail du réseau RMN structurale dans le Grand Bassin Parisien, Rennes (France), January 2012

12. *Application of Machine Learning Algorithms to the study of atomic and molecular aggregats*
    J. Cuny, G. A. Tribello, M. Parrinello
    CECAM Workshop on Machine Learning in Atomistic Simulations, Lugano (Switzerland), September 2012

13. *Mise en évidence et caractérisation des effets quantiques nucléaires en phase condensée*
    J. Cuny, A. A. Hassanali, M. Ceriotti, M. Deschamps, M. Parrinello
    GDR CoDFT 2013, Guidel Plages (France), May 2013

14. *New Molecular Dynamics Approaches to Model Activated Processes and Nuclear Quantum Effects: Implementation in the deMon-nano Code*
    J. Cuny
    deMon Workshop 2013, Toulouse (France), June 2013

15. *Développements et utilisation de la méthode Density Functional based Tight-Binding pour la simulation moléculaire*
    J. Cuny, F. Spiegelman, A. Scemama, M. Rapacioli, A. Simon, L. Dontot, L. Oliveira, K. Korchagina
    82e Congrès de l'Acfas, Montréal (Canada), May 2014

16. *Implementation in deMon-nano of new thermostats based on stochastic equations of motion: application to the simulation of heat capacity curves and liquid water*
    J. Cuny, M. Rapacioli, A. Simon, F. Spiegelman
    deMon Workshop 2015, Sofia (Bulgaria), May 2015

17. *Structural, dynamical and thermodynamical properties of ion-containing water clusters*
    K. Korchagina, J. Cuny, A. Simon, M. Rapacioli, F. Spiegelman
    deMon Workshop 2015, Sofia (Bulgaria), May 2015

18. *Propriétés structurales, dynamiques et thermodynamiques de clusters de molécules d'eau*
    J. Cuny, K. Korchagina, L. F. Oliveira, M. Rapacioli, A. Simon, F. Spiegelman
    Journées Dynamiques du Sud-Ouest 2015, Toulouse (France), June 2015

19. *Etude par dynamique moléculaire de la recombinaison de H et CO à la surface de clusters d'eau*
    K. Korchagina, J. Cuny et F. Spiegelman
    GDR EMIE – Réunion plénière 2015, Biarritz (France), May-June 2015

20. *Caractérisation structurale, thermodynamique et dynamique des agrégats de molécules d'eau contenant des espèces sulfurées*
    K. Korchagina, J. Cuny, A. Simon, M. Rapacioli, F. Spiegelman
    TouCAM 2015 – Toulousaines du Calcul Atomique et Moléculaire, Toulouse (France), Novembre 2015

21. *First steps towards the implementation of metadynamics and path-integral molecular dynamics in deMon2k*
    J. Cuny and Tzonka Mineva
    deMon Workshop 2016, Zhengzhou (China), May 2016

22. *Structure and Reactivity of Octahedral Molybdenum Clusters in Aqueous Solution Probed by Molecular Dynamics*
J. Cuny, X. Trivelli, S. Cordier, Y. Molard, R. Gautier
CLUSPOM-1, Rennes (France), June-July 2016

23. *Molecular Dynamics Study of the Structure and Reactivity of Ruthenium Polypyridine Complexes in Aqueous Solution*
J. C*uny*, *A. J. Göttle, I. M. Dixon, F. Alary*
42nd International Conference on Coordination Chemistry (ICCC 2016), Brest (France), 3-8 July 2016

24. *Transition Metal Clusters as Building Blocks for Multifunctional Proton-Conducting Materials*
G. Daigre, **J. Cuny**, P. Lemoine, M. Amela-Cortes, S. Paofai, N. Audebrand, A. le Gal La Salle, E. Quarez, O. Joubert, N. G. Naumov, S. Cordier
International Workshop on Transition Metal Clusters, Tübingen (Germany), 5-7 September 2018

25. *Transition Metal Clusters as Building Blocks for Multifunctional Proton-Conducting Materials*
G. Daigre, **J. Cuny**, P. Lemoine, M. Amela-Cortes, S. Paofai, N. Audebrand, A. le Gal La Salle, E. Quarez, O. Joubert, N. G. Naumov, S. Cordier
19th Solid State Protonic Conductors, Stowe (Vermont U.S.A), 16-21 September 2018

26. *Développements et applications de l'approche SCC- DFTB pour la chimie atmosphérique*
J. Cuny K. Korchagina, M. Rapacioli, F. Spiegelman and A. Simon
Atelier Conjoint des GDRs Suie et EMIE, Lille University, May 31st - June 1st 2018

27. *Size-Dependent Proton Localization in Hydrated Uracil Clusters: a Joint Experimental and Theoretical Study*
I. Braud, S. Zamith, J. Cuny, **L. Zheng**, J.-M. L'Hermite
GDR EMIE - Réunion plénière 2018, Nouan-le-Fuzelier (France), 12-15 November 2018

28. *Parallel-Tempering Path-Integral Molecular Dynamics Approach to Water Clusters Simulations*
F. Louisnard, A. Simon, J. Cuny
deMon Workshop 2019, Frejus (France), May 2019

29. *Size-dependent proton localization in hydrated uracil clusters*
L. Zheng, M. Rapacioli, F. Louisnard, I. Braud, S. Zamith, J.-M. L'Hermite, J. Cuny
TOUCAM 2019, Toulouse (France), November 7-8 2019

30. *Synchronous and Asynchronous implementation of the Parallel-Tempering Molecular Dynamics method in the codes deMonNano and deMon2k*
F. Louisnard, A. Simon, J. Cuny
TOUCAM 2019, Toulouse (France), November 7-8 2019

INVITED SEMINAR - TUTORIALS

1. *First-Principles Calculations of ^{95}Mo NMR Parameters in Insulating Diamagnetic Solid-State Compounds*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye
Workshop NMR spectroscopy and electronic structure calculations, Dresden (Germany), March 2009

2. *Solid State ^{95}Mo NMR and Modelling: Converging Tools for New Material Development*
J. Cuny, R. Gautier, L. Le Pollès, C. J. Pickard, J. Trebosc, L. Delevoye
Magnetic Resonance Seminar, St. Andrews (England), February 2010

3. *Solid State ^{95}Mo NMR and Modelling: Converging Tools for the Development of New Materials*
J. Cuny, L. Le Pollès, R. Gautier, C. J. Pickard, J. Trebosc, L. Delevoye
Equipe de M. Parrinello, ETH, Lugano (Switzerland), March 2010

4. *^{95}Mo Solid-State NMR Study of Transition Metal Cluster Compounds: A Synergetic Experimental and Computational Approach*
J. Cuny, R. Gautier, L. Le Pollès, C. J. Pickard, J. Trebosc, L. Delevoye
Séminaire Groupement Scientifique RMN - Nord Pas de Calais, Université Lille 1, Lille (France), July 2010

5. *Dynamique moléculaire, metadynamics et RMN en phase solide : approches convergentes pour l'étude de différentes problématiques chimiques*
J. Cuny, R. Gautier, L. Le Pollès, Y. Xue, A. A. Hassanali, C. J. Pickard, M. Parrinello

Equipe UCCS, Université de Lille 1, Lille (France), February 2012

6. *Dynamique moléculaire, metadynamics et RMN en phase solide : approches convergentes pour l'étude de différentes problématiques chimiques*
   J. Cuny, R. Gautier, L. Le Pollès, Y. Xue, A. A. Hassanali, C. J. Pickard, M. Parrinello
   CEMHTI-CNRS, Orléans (France), February 2012

7. *Applications de la dynamique moléculaire et de la metadynamics aux aspects dynamiques des propriétés RMN et à la réactivité en solution*
   J. Cuny, R. Gautier, L. Le Pollès, Y. Xue, A. A. Hassanali, C. J. Pickard, M. Parrinello
   Sciences Chimiques de Rennes, Université de Rennes 1, Rennes (France), March 2012

8. *Metadynamics : principes, utilisation et applications à l'étude de composés à clusters de métaux de transition*
   J. Cuny, R. Gautier, S. Cordier, Y. Molard, X. Trivelli
   Sciences Chimiques de Rennes, Université de Rennes 1, Rennes (France), February 2013

9. *Metadynamics and Path-Integral Molecular Dynamics, Two Theoretical Approaches to Study Hydrogen Reactivity in the Interstellar Medium*
   J. Cuny, G. Tribello, M. Ceriotti, M. Deschamps, M. Parrinello
   Atelier H_2/Grains de l'AST Molécules et Grains, Toulouse (France), April 2013

10. *Density-Functional based Tight-Binding : application à la description dynamique et thermodynamique des systèmes chimiques*
    J. Cuny, L. Dontot, M. Rapacioli, A. Simon, L. Oliveira, K. Korchagina, F. Spiegelman
    Sciences Chimiques de Rennes, Université de Rennes 1, Rennes (France), April 2014

11. *SCC-DFTB Modelling of the Carbonyl-Hydrogen Recombination on Water Aggregates: Toward the Formation of Complex Oxygenated Molecules*
    K. Korchagina, **J. Cuny**, A. Simon, M. Rapacioli, F. Spiegelman
    NANOCOSMOS Theoreticians Meeting 2015, Toulouse (France), December 2015

12. *Utilisation de l'approche self-consistent-charge density-functional based tight- binding (SCC-DFTB) pour la modélisation de processus astro-chimiques*
    J. Cuny, A. Simon, M. Rapacioli, K. Korchagina, F. Spiegelman
    LAMPS, Perpignan (France), March 2016

13. *Enhanced Sampling Methods for Improving Molecular Dynamics Simulations*
    J. Cuny
    deMon2k and deMonNano Tutorial, Zhengzhou (China), May 2016

14. *Contribution of DFT and DFTB Methods to the Description of Aqueous Systems from Water Clusters to Condensed Matter Systems*
    J. Cuny and K. Korchagina
    Journée des Jeunes Chercheurs, Département de Chimie - Ecole Polytechnique, January 2017

15. *Exploration of Potential Energy Surfaces - Molecular Dynamics*
    J. Cuny
    TCCM Winter School 2017-2019, Tutorials in Theoretical Chemistry, Luchon (France), January 2017-2019

16. *Contribution of the DFTB Method to Describe Aqueous Systems: From Water Clusters to Condensed Matter Systems*
    J. Cuny, K. Korchagina, M. Rapacioli, F. Spiegelman, A. Simon
    ICTP - Condensed Matter Section Seminar, Trieste (Italy), November 2018

17. *Contribution of the DFTB Method to Describe Aqueous Systems: From Water Clusters to Condensed Matter Systems*
    J. Cuny, K. Korchagina, M. Rapacioli, F. Spiegelman, A. Simon
    Queen's University, Belfast (North Ireland), February 2020

STUDENT SUPERVISION

PhD STUDENTS

- **Thi Thuong Nguyen (2011-2015)** PhD: "First-Principles Calculations of Solid- State Transition Metal NMR Parameters in Inorganic Materials" (Co-supervisor).
- **Kseniia Korchagina (2013-2016)** PhD: "Molecular Dynamics Study of the Structural, Dynamical and Thermodynamical Properties of Molecular Clusters" (Co-supervisor, 50%).
- **Carles Marti Aliod (2015-2018)** PhD: "Networked Computing for ab initio modeling the chemical storage of alternative energy » (Co-supervisor, 20%).
- **Linjie Zheng** (**2017-2021**) PhD: "Excited States and Solvatochromism Properties of Large Organic Molecules: from *in vivo* cell imaging to dye-sensitized solar cells" (Supervisor).
- **Fernand Louisnard** (**2018-2021**) PhD: "Energy Landscapes and Nuclear Quantum Effects: Parallel-Tempering Path-Integral Molecular Dynamics Approach" (Co-supervisor, 50%).
- **Nicolas Cinq** (**2019-2022**) PhD: "Influence of Impurities on Water-(solvant/gas hydrate) Interfaces Probed by Molecular Dynamics » (Co-supervisor, 50%)

MASTER STUDENTS

- **Maxime Morinière (2013)** Master 2 training period: "A*b initio* molecular dynamic study of the hydrogen addition on carbon monoxide on water clusters" (Supervisor).
- **Arthur Huguenot** (**2016**) Master 1 training period: "Structural, dynamical and thermodynamics properties of methanol clusters" (Supervisor).
- **Fernand Louisnard** (**2017**) Master 1 training period: "Computational Study of Water Clusters containing Ammoniac and Ammonium" (Supervisor).
- **Kanishka Singh** (**2019**) Master 2 training period: "Reactive Potential Energy Surfaces: Fitting with Gaussian Process Regression" (Co-Supervisor).
- **Azahara Doncel** (**2020**) Master 2 training period: "Computational strategies to estimate the self-assembly free energy in supramolecular polymers" (Co-Supervisor).

BACHELOR STUDENTS

- **Fernand Louisnard, Mélani Centenero, Matilda Delgado, Maxime Ferrer, Amélie Icher, Mélissa Bonnet,** *Training period for L2 Parcours Spéciaux*.

AWARDS

- Award winner of the «Prix Gineste de Chimie 2011», prize awarded by the University of Rennes 1 Foundation.
- Recipient of the PEDR 2016-2020 (prime d'encadrement doctoral et de recherche)

ORGANIZATION OF SCIENTIFIC MEETINGS

- DeMon Workshop 2013, Toulouse, France
- TCCM Winter Schools 2017 and 2018, School for advanced sciences of Luchon, Luchon-Superbagnères, France
- 16ème Rencontre des Chimistes Théoriciens Francophones (RCTF 2018), Toulouse, France
- DeMon Workshop 2019, Fréjus, France
- Multidisciplinary Summerschool on Nanosciences and Nanotechnologies 2020 (NanoX Graduate School of Research), Toulouse, France.

SCIENTIFIC NETWORK

- ANR (French National Agency for Research) grant n°ANR-13-BS08-0005 PARCS
- ERC (European Research Council) grant Nanocosmos (ERC-2013-SyG Grant Agreement nº 610256)
- ANR (French National Agency for Research) grant n°ANR-16-CE29-0025 PACHYNO
- ANR (French National Agency for Research) grant n°ANR-18-CE05-0028 MUSCOFI
- ANR (French National Agency for Research) grant n°ANR-19-CE29-0008-01 ZEOORG

COLLECTIVE RESPONSIBILITIES

- Webmaster of the LCPQ website (2015-now)
- Member at the Laboratory Council of the LCPQ (2016-now)
- Member of the doctoral school board «Sciences de la matière»
- Elected Member at the Chemistry Department Council and Member of the Board (2016-2021)
- Appointed Member at the Chemistry Scientific Group of the UPS (2018-2021)
- Elected Member at the Training and University Life Committee of UPS (2020-2024)
- Elected Member at the Academic Council of UPS (2020-2024)
- Elected Member at the Disciplinary Commission of UPS (2020-2024)