

Curriculum Vitae

(Update: October 2022)

Loïc Joubert-Doriol

**Maître de Conférences (assistant prof.), Université Gustave Eiffel (UGE)
Section CNU 31**

Contact: Laboratoire Modélisation et Simulation Multi Échelle, équipe Chimie Théorique
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Scientific interests:

Theoretical chemistry, simulation, **photochemistry**, **non-adiabatic quantum dynamics**, **open systems**, curvilinear coordinates, **“on-the-fly” quantum dynamics** with Gaussian basis.

Education:

2009-2012 **PhD in Theoretical Chemistry**, Université de Montpellier, France.

2007-2009 **Master degree in Chemical Physics and Theoretical Chemistry** (label de chimie théorique), Université Joseph Fourier, Grenoble, France.

2006-2007 Bachelor degree in Chemistry and Physics, Université Joseph Fourier, Grenoble, France.

2003-2006 Bachelor degree in Chemistry and Biology, Université Joseph Fourier, Grenoble, France.

Academic employments:

Since Sep 2018: **Maître de Conférences (assistant prof.), Université Gustave Eiffel**,
in the group Chimie Théorique (CT) of the laboratory Modélisation et Simulation
Multi Échelle (MSME),
and teaching at the Institut Francilien des Sciences Appliqués (IFSA)

2016-2018: **Postdoctoral fellow: University of Toronto in the group of Prof. Artur Izmaylov**,
developing novel “on-the-fly” Quantum Dynamics approaches

2013-2016: **Marie-Curie international postdoctoral fellow (European)**,
Project FP7-MC-IOF-332233 PinadBIO

Title: First Principles Study of Photo-induced Non-Adiabatic Dynamics in DNA
Repair Photolyases

Supervisors: **Artur Izmaylov**, University of Toronto, Canada, Jan. 2013 to March 2015 ;
Massimo Olivucci, University of Siena, Italy, April 2015 to March 2016.

2009-2012: **PhD: National French Scholarship (“contrat doctoral”)**

Title: Control of organic photochemistry. Theoretical strategy coupling quantum chemistry and quantum dynamics

Supervisors: **Fabien Gatti** and **Benjamin Lasorne**, universit  Montpellier 2, Montpellier, France.

Jan.-Jun. 2009: **Second year Master project**

Title: Time-Dependent Density Functional Theory for open shell molecules

Supervisor: **Mark Casida**, Joseph Fourier University, Grenoble, France.

Teaching experience:

Since 2018 **Maître de Conférences**, Université Gustave Eiffel, France.

Classical Mechanics	Course / tutorial / Lab	1 st year	34 h / 34 h / 8 h	2018-2022
Numerical Methods	Tutorial / Lab	3 rd year	30 h	2018-2022
Wave Optics	Course / tutorial / Lab	1 st year	6 h / 8 h / 12 h	2019-2020, 2022
Quantum Mechanics	Course / tutorial	3 rd year	12 h / 12 h	2021

2009-2012 **Teaching** (“Mission complémentaire d'enseignement”), University of Nîmes, France.

Thermochemistry	Tutorial	1 st / 2 nd year	44 h / 10 h
Conductimetry	Course and Tutorial	1 st year	10 h
Inorganic Chemistry	Lab	1 st / 2 nd year	24 h / 40 h
Analytical Chemistry	Lab	2 nd year	48 h
Thermochemistry	Lab	3 rd year	20 h

2008 **Tutor of a 3rd year student**, University Joseph Fourier, Grenoble, France.

Students supervision and co-supervision:

Dates	Name	Place	Co-supervisor	Level
Apr – Jun 2009	Sébastien Bruneau	Université Joseph Fourier, Grenoble	Mark Casida	Master 2 nd y
Sept 2011 – Sept 2012	Mohamad Saab	Université Montpellier 2	Fabien Gatti	PhD
May 2013 – Feb 2014	Syed Ather Hasnain Rizvi	University of Toronto, Canada	Artur Izmaylov	Bachelor
Nov 2016 – May 2017	Jiaru Li			Bachelor
Aug 2017 – Jul. 2018	Mina Asaad			Master

Apr – Jun 2019	Rémi Vançon	Université Paris-Est Marne-la-Vallée, Champs-sur-Marne		Master 1 st y
May – Jun 2019				Master 1 st y
Feb – Aug 2020	Rosa Maskri	L'Oréal, Aulnay-sous-Bois	Jérôme Gomar	Master 2 nd y
Since Oct 2020		Université Gustave Eiffel, Champs-sur-Marne	Isabelle Navizet	
			Alexander Mitrushchenkov	PhD
Mar – Jun 2021	David Nishimwe	Université Gustave Eiffel, Champs-sur-Marne	Étienne Mangaud	Bachelor
Since Jan 2022	Kossi Kety	Université Gustave Eiffel, Champs-sur-Marne	Alexander Mitrushchenkov	PhD
Mar – Jul 2022	Mina Asaad	Université de Toronto, Canada	Artur Izamylov	PhD

Grants and Awards:

- 2021-2025 **Scientific leader** for the MSME partner in the “**Agence National pour la Recherche**” (ANR) grant for the project AttoChemistry
“Chemistry with attosecond pulses: inducing charge migration and charge transfer in small biomolecules”, coordinated by Fabien Gatti.
Funding for Kossi Kety’s PhD.
- 2013-2016 **European Fellowship** for postdoctoral research:
Funded by the **Seventh Framework Programme: Marie-Curie IOF**
“First Principles Study of Photo-induced Non-Adiabatic Dynamics in DNA Repair Photolyases”
- Aug 2014 **Poster prize:** *“Geometric phase effects in multidimensional quantum dynamics near conical intersections”*
L. Joubert-Doriol, I. G. Ryabinkin, and A. F. Izmaylov
XXIInd International Symposium on the Jahn-Teller Effet, Graz, Austria.
- Jul 2011 **Poster prize:** *“An investigation of photochemical the ring-opening of benzopyran”*
L. Joubert-Doriol, B. Lasorne, and F. Gatti
Ninth triennial Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain.
- 2009-2012 **National French scholarship** for PhD thesis:
“Doctorant Contractuel avec Mission Complémentaire d'Enseignement”,
“Control of organic photochemistry. Theoretical strategy coupling quantum chemistry and quantum dynamics”

Publications:

25 articles, 803 citations, h-index: 14 (source: Google Scholar). Selection of 5 articles :

- 1) [L. Joubert-Doriol](#), “Variational Approach for Linearly Dependent Moving Bases in Quantum Dynamics: Application to Gaussian Functions”, *J. Chem. Theory Comput.* **18**, 5799 (2022).
- 2) R. Masrkri and [L. Joubert-Doriol](#), “The moving crude adiabatic alternative to the adiabatic representation in excited state dynamics”, *Phil. Trans. R. Soc. A* **380**, 20200379 (2018).
- 3) [L. Joubert-Doriol](#) and A. F. Izmaylov, “Nonadiabatic Quantum Dynamics with Frozen-Width Gaussians”, *J. Phys. Chem. A* **122**, 6031 (2018). **Feature article and cover.**
- 4) [L. Joubert-Doriol](#), J. Sivasubramaniam, I. G. Ryabinkin and A. F. Izmaylov, “Topologically correct quantum nonadiabatic formalism for on-the-fly dynamics”, *J. Phys. Chem. Lett.* **8**, 452 (2017).
- 5) I. G. Ryabinkin, [L. Joubert-Doriol](#) and A. F. Izmaylov, “Geometric Phase Effects in Nonadiabatic Dynamics near Conical Intersections”, *Acc. Chem. Res.* **50**, 1785 (2017).

Communications:

13 invited talks and seminars; 13 contributed talks; 19 posters. Selection of 5 communications:

- 1) **Waves 2022**, Jul 2022. “Quantum dynamics beyond the Born-Oppenheimer approximation in molecular systems”, [L. Joubert-Doriol](#)
- 2) **5th meeting GDR Ultrafast Phenomena**, Nov 2021. “Should we abandon adiabatic states to describe ultrafast molecular dynamics?”, [L. Joubert-Doriol](#)
- 3) **Watching Chemistry Happen**, online, Apr 2021. “Is the time-dependent variational principle really adapted for independent moving Gaussians?”, [L. Joubert-Doriol](#)
- 4) **Working Group 2 Workshop of the COST Action CA18222**, online, Feb 2021. “From low-energy nonadiabatic dynamics to attochemistry”, [L. Joubert-Doriol](#)
- 5) **Conference on Light and Molecules**, Marseille, France, Oct 2019. “The moving crude adiabatic representation: how to use adiabatic states for non-adiabatic dynamics?”, [L. Joubert-Doriol](#).

Administratives activities:

Mar-Jun 2022	Organizing committee of the Social day of the “Modélisation et Simulation Multi Echelle” laboratory (“ Journée MSME 2022 ”) to be held in June 2022.
Since Oct 2021	Elected member of the chemistry standing committee at “Université Gustave Eiffel” (related to the CNU section 31).
Since Sept 2021	International contact (“ Correspondant international ”) for the “Modélisation et Simulation Multi Echelle” laboratory.
Apr-May 2020	Member of the selection committee for an assistant professor (“Maître de conférences”) position at “Université Gustave Eiffel”.
Since Feb 2020	Elected member of the “Modélisation et Simulation Multi Echelle” laboratory Council board (“ Conseil du laboratoire MSME ”).

Computational skills:

Quantum Chemistry / Dynamics:

Gaussian User of Complete Active Space Self Consistent Field method (CASSCF)

DeMon2k Time-Dependent Density Functional Theory (TDDFT): “Davidson” diagonalization and excited states spin contamination

Molcas, Molpro, Firefly User of CASSCF and perturbative post-CASSCF methods (**CASPT2, XMCQDPT2**)

MCTDH/Quantics User of the **propagation** and **improved relaxation** methods

Other: script Shell, Matlab / **Octave, Fortran, MPI**, Linux/Windows operating systems, LaTeX

Attended courses:

Apr 2013 Rome School on Open Systems and the Quantum-Classical Boundary at University of Rome La Sapienza, Italy.

Mar 2010 NBO course by Clark Landis at University of Montpellier France.

2008-2009 Theoretical Chemistry courses, “Réseau Français de Chimie Théorique”, Lyon (2008) and Grenoble (2009), France.

Outreach activities:

Oct, 2020-22 Volunteer at “**fête de la science**”, Lavoisier, Champs-sur-Marne.

Jan 17, 2015 Volunteer at the “Brain Fest” **festival**, Ontario Sciences Center, Toronto, Canada.

May 10, 2014 Volunteer at “Science Rendezvous” **festival**, University of Toronto, Canada.

2014-2015 **Member of the outreach organisation** “Let's Talk Science”.

2006-2007 **Activity leader** at “centre culturel, scientifique et industriel” (CCSTI) of Grenoble, France, including the “**fête de la science 2007**” festival in Grenoble.

Detailed list of scientific productions

Articles: (26)

- A26 [L. Joubert-Doriol](#), “Variational Approach for Linearly Dependent Moving Bases in Quantum Dynamics: Application to Gaussian Functions”, *J. Chem. Theory Comput.* **18**, 5799 (2022).
- A25 M. Asaad, [L. Joubert-Doriol](#), and A. F. Izmaylov, “Controlling energy conservation in quantum dynamics with independently moving basis functions: Application to Multi-Configuration Ehrenfest”, *J. Chem. Phys.* **156**, 204121 (2022).
- A24 R. Maskri and [L. Joubert-Doriol](#), “The moving crude adiabatic alternative to the adiabatic representation in excited state dynamics”, *Phil. Trans. R. Soc. A* **380**, 20200379 (2022).
- A23 B. Gonon, B. Lasorne, G. Karras, [L. Joubert-Doriol](#), D. Lauvergnat, F. Billard, B. Lavorel, O. Faucher, S. Guérin, E. Hertz and F. Gatti, “A generalized vibronic-coupling Hamiltonian for molecules without symmetry: Application to the photoisomerization of benzopyran”, *J. Chem. Phys.* **150**, 124109 (2019).
- A22 [L. Joubert-Doriol](#) and A. F. Izmaylov, “Nonadiabatic Quantum Dynamics with Frozen-Width Gaussians”, *J. Phys. Chem. A* **122**, 6031 (2018). **“Feature article”** and **cover**.
- A21 [L. Joubert-Doriol](#) and A. F. Izmaylov, “Variational nonadiabatic dynamics in the moving crude adiabatic representation: Further merging of nuclear dynamics and electronic structure”, *J. Chem. Phys.* **148**, 114102 (2018).
- A20 H. Daoud, [L. Joubert-Doriol](#), A. F. Izmaylov and R. J. D. Miller, “Exploring vibrational ladder climbing in vibronic coupling models: Toward experimental observation of a geometric phase signature of a conical intersection”, *Chem. Phys.* **515**, 28 (2018).
- A19 [L. Joubert-Doriol](#), J. Sivasubramanium, I. G. Ryabinkin, and A. F. Izmaylov, “*Topologically correct quantum nonadiabatic formalism for on-the-fly dynamics*”, *J. Phys. Chem. Lett.* **8**, 452 (2017).
- A18 [L. Joubert-Doriol](#) and A. F. Izmaylov, “Molecular “*Topological Insulator*”: A Case Study of *Electron Transfer in Bis (Methylene) Adamantyl Carbocation*”, *Chem. Commun.* **53**, 7365 (2017).
- A17 I. G. Ryabinkin, [L. Joubert-Doriol](#), and A. F. Izmaylov, “Geometric Phase Effects in Nonadiabatic Dynamics near Conical Intersections”, *Acc. Chem. Res.* **50**, 1785 (2017).
- A16 A. F. Izmaylov and [L. Joubert-Doriol](#), “*Quantum Nonadiabatic Cloning of Entangled Coherent States*”, *J. Phys. Chem. Lett.* **8**, 1793 (2017).
- A15 J. Li, [L. Joubert-Doriol](#), and A. F. Izmaylov, “Geometric phase effects in excited state dynamics through a conical intersection in large molecules: N-dimensional linear vibronic coupling model study”, *J. Chem. Phys.* **147**, 064106 (2017).

- A14 A. F. Izmaylov, J. Li, and L. Joubert-Doriol, “Diabatic Definition of Geometric Phase Effects”, *J. Chem. Theory Comput.* **12**, 5278 (2016).
- A13 L. Joubert-Doriol, and A. F. Izmaylov, “Problem-free time-dependent variational principle for open quantum systems”, *J. Chem. Phys.* **142**, 134107 (2015).
- A12 L. Joubert-Doriol, I. G. Ryabinkin, and A. F. Izmaylov, “Non-stochastic matrix Schrödinger equation for open systems”, *J. Chem. Phys.* **141**, 234112 (2014).
- A11 M. Saab, L. Joubert Doriol, B. Lasorne, S. Guérin, and F. Gatti, “A quantum dynamics study of the benzopyran ring opening guided by laser pulses”, *Chem. Phys.* **442**, 93 (2014).
- A10 J. S. Endicott, L. Joubert-Doriol, and A. F. Izmaylov, “A perturbative formalism for electronic transitions through conical intersections in a fully quadratic vibronic model”, *J. Chem. Phys.* **141**, 034104 (2014).
- A9 I. G. Ryabinkin, L. Joubert-Doriol, and A. F. Izmaylov, “When do we need to account for the geometric phase in excited state dynamics?”, *J. Chem. Phys.* **140**, 214116 (2014). **2014 Editor's choice.**
- A8 L. Joubert-Doriol, B. Lasorne, D. Lauvergnat, H.-D. Meyer, and F. Gatti, “A generalised vibronic-coupling Hamiltonian model for benzopyran”, *J. Chem. Phys.* **140**, 044301 (2014).
- A7 L. Joubert-Doriol, I. G. Ryabinkin, and A. F. Izmaylov, “Geometric phase effects in low-energy dynamics near conical intersections: A study of the multidimensional linear vibronic coupling model”, *J. Chem. Phys.* **139**, 234103 (2013).
- A6 M. Ndong, A. Nauts, L. Joubert-Doriol, H.-D. Meyer, F. Gatti, and D. Lauvergnat, “Automatic computer procedure for generating exact and analytical kinetic energy operators based on the polyspherical approach: General formulation and removal of singularities”, *J. Chem. Phys.* **139**, 204107 (2013).
- A5 L. Joubert-Doriol, B. Lasorne, F. Gatti, M. Schröder, O. Vendrell, and H.-D. Meyer, “Suitable Coordinates for Quantum Dynamics: Applications”, *Comp. Theo. Chem.* **990**, 75 (2012).
- A4 M. Ndong, L. Joubert-Doriol, H.-D. Meyer, A. Nauts, F. Gatti, and D. Lauvergnat, “Automatic computer procedure for generating exact and analytical kinetic energy operators based on the polyspherical approach”, *J. Chem. Phys.* **136**, 034107 (2012).
- A3 A. Ipatov, F. Cordova, L. Joubert Doriol, and M. E. Casida, “Excited-State Spin-Contamination in Time-Dependent Density-Functional Theory for Molecules with Open-Shell Ground States”, *Theochem* **914**, 60 (2009).
- A2 L. Joubert Doriol, F. Gatti, C. Iung, and H.-D. Meyer, “Computation of vibrational energy levels and eigenstates of fluorofom using the multiconfiguration time-dependent Hartree method”, *J. Chem. Phys.* **129**, 224109 (2008).
- A1 F. Cordova, L. Joubert Doriol, A. Ipatov, M. E. Casida, C. Fillipi, and A. Vela, “Troubleshooting Time-Dependent Density Functional Theory for Photochemical

Applications: Oxirane”, *J. Chem. Phys.* **127**, 164111 (2007).

Submitted paper :

L. Joubert-Doriol, K. A. Jung, A. Izmaylov, and P. Brumer, “Quantum Kinetic Rates within the Nonequilibrium Steady State”, arXiv:2209.01154 [quant-ph] (2022), <https://doi.org/10.48550/arXiv.2209.01154>, submitted to *J. Chem. Theory Comput.* (2022).

Invited talks and seminars : (13)

- I13 **Waves 2022**, Jul 2022. “Quantum dynamics beyond the Born-Oppenheimer approximation in molecular systems”, L. Joubert-Doriol
- I12 **5th meeting GDR Ultrafast Phenomena**, Nov 2021. “Should we abandon adiabatic states to describe ultrafast molecular dynamics?”, L. Joubert-Doriol
- I11 **Quantum Dynamics Network meeting**, Sep 2021. “Chemistry with attosecond pulses: inducing charge migration and charge transfer in small biomolecules”, L. Joubert-Doriol
- I10 **Watching Chemistry Happen**, online, Apr 2021. “Is the time-dependent variational principle really adapted for independent moving Gaussians?”, L. Joubert-Doriol
- I9 **Working Group 2 Workshop of the COST Action CA18222**, online, Feb 2021. “From low-energy nonadiabatic dynamics to attochemistry”, L. Joubert-Doriol
- I8 Seminar: CFL-DESY, Centre for Free electron Laser science, Hambourg, Oct 2020. “Nonadiabatic quantum dynamics with frozen-width Gaussians”, L. Joubert-Doriol
- I7 **Conference on Light and Molecules**, Marseille, France, Oct 2019. “The moving crude adiabatic representation: how to use adiabatic states for non-adiabatic dynamics?”, L. Joubert-Doriol
- I6 **Mathematical Questions of Molecular Quantum Dynamics**, Paris, France, Sep 2019. “Understanding and accounting for geometric phase effects in direct dynamics near conical intersections”, L. Joubert-Doriol
- I5 Seminar: LCT, laboratoire Modélisation et Simulation Multi Échelle, Champs-sur-Marne, France, May 2018. “Dynamique moléculaire au-delà de l’approximation de Born-Oppenheimer: la phase géométrique”, L. Joubert-Doriol.
- I4 Seminar: Department of Chemistry, Université McGill, Montréal, Canada, Mar 2018. “Geometric phase effects in molecular dynamics beyond the Born-Oppenheimer approximation”, L. Joubert-Doriol.
- I3 Seminar: THEO, Institut des Sciences Moléculaires, Bordeaux, France, Oct 2016. “Describing non-adiabatic quantum effects in large systems”, L. Joubert-Doriol.
- I2 Seminar : LCQ, Institut de chimie, Strasbourg, France, Oct 2015. “Towards computational non-

adiabatic biology: Methods et application to the DNA repair”, L. [Joubert-Doriol](#).

- I1 Seminar: CTMM, ICGM, Montpellier, France, Sep 2014. “Geometric phase effects on the dynamics of molecular systems in the neighbourhood of a conical intersection”, [L. Joubert-Doriol](#), I. G. Ryabinkin, et A. F. Izmaylov.

[Contributed talks and other seminars](#) : (13)

- O13 **Journées GDR ThÉMS**, Orsay, France, Nov 2019. “Utilizing adiabatic states in Non-adiabatic direct quantum dynamics”, [L. Joubert-Doriol](#)
- O12 **Journée scientifique MSME**, Champs-sur-Marne, France, Jun 2019. “Dynamiques couplées des électrons et des noyaux pour la photochimie des systèmes moléculaires”, [L. Joubert-Doriol](#)
- O11 **Journées Théorie, Modélisation et Simulation**, Paris, France, Jun 2019. “The moving crude adiabatic representation to avoid conical intersection-related problems in "on-the-fly" quantum dynamics”, [L. Joubert-Doriol](#)
- O10 **High Dimensional Quantum Dynamics**, Lille, France, Aug 2018. “Direct quantum nonadiabatic dynamics in the moving crude adiabatic representation”, [L. Joubert-Doriol](#) et A. F. Izmaylov
- O9 **Quantum Dynamics: from Algorithms to Applications**, Greifswald, Germany, Sep 2016. “Geometric phase in multidimensional quantum dynamics”, [L. Joubert-Doriol](#), I. G. Ryabinkin, et A. F. Izmaylov
- O8 **High Dimensional Quantum Dynamics**, Rostock, Germany, Sep 2016. “Conical intersection induced interference in multidimensional quantum dynamics”, [L. Joubert-Doriol](#), I. G. Ryabinkin, et A. F. Izmaylov
- O7 **249th ACS National Meeting**, Denver, USA, Mar 2015. “Theoretical study of the electron transfer in DNA repair process of the cyclobutane pyrimidine dimer lesion”, [L. Joubert-Doriol](#), T. Domratcheva, M. Olivucci, et A. F. Izmaylov.
- O6 **2014 Symposium on Chemical Physics**, Waterloo, Canada, Oct 2014. “Problem-free Time-Dependent Variational Principle for Open quantum Systems”, [L. Joubert-Doriol](#), I. G. Ryabinkin, et A. F. Izmaylov.
- O5 **High Dimensional Quantum Dynamics**, Mittelwihr, France, Sep 2014. “A Constrained Time-Dependent Variational Principle for Open Systems”, [L. Joubert-Doriol](#), I. G. Ryabinkin, et A. F. Izmaylov.
- O4 **Rencontre des Chimistes Théoriciens Francophones**, Marseille, France, Jul 2012. “Élaboration d'un modèle théorique pour décrire l'ouverture photochimique du benzopyrane”, [L. Joubert-Doriol](#), B. Lasorne, H.-D. Meyer, et F. Gatti.
- O3 **Journée des Chimistes Théoriciens de l'ICG**, Grabels, France, Jun 2012. “Élaboration d'une stratégie pour la construction de modèles de surfaces d'énergie potentielle : application à l'ouverture du benzopyrane”, [L. Joubert-Doriol](#), B. Lasorne, et F. Gatti.

- O2 **Les journées de l'ICGM**, Teyran, France, Mar 2011. “Contrôle de la photochimie organique. Élaboration d'une stratégie couplant chimie quantique et dynamique quantique”, L. Joubert-Doriol, B. Lasorne, et F. Gatti.
- O1 **Rencontre des Chimistes Théoriciens Francophones**, Namur, Belgium, Jul 2010. Flash presentation: “Étude théorique de l'ouverture du benzopyrane application au contrôle photochimique”, L. Joubert-Doriol, B. Lasorne, et F. Gatti.

Communications par affiches : (19)

- P19 High Dimensional Quantum Dynamics, Groningen, Nederland, Jul 2022.
- P18 First meeting of GDR NBODY, Lille, France, Jan 2020.
- P17 2017 Symposium on Chemical Physics, Waterloo, Canada, Nov 2017.
- P16 100th Canadian Chemistry Conference and Exhibition, Toronto, Canada, May 2017.
- P15 2016 Symposium on Chemical Physics, Waterloo, Canada, Nov 2016.
- P14 Rencontre des Chimistes Théoriciens Francophones, Lyon, France, Jul 2016.
- P13 DNA damages: modeling and rationalize structure and reactivity, Lyon, France, Nov 2015.
- P12 Modelling Photoactive Molecules Conference, Nantes, France, Apr 2015.
- P11 XXIInd International Symposium on the Jahn-Teller Effect, Graz, Austria, Aug 2014. **Prix du poster**: “Geometric phase effects in multidimensional quantum dynamics near conical intersections”, L. Joubert-Doriol, I. G. Ryabinkin, et A. F. Izmaylov.
- P10 26th Canadian Symposium on Theoretical et Computational Chemistry, Montréal, Canada, Jul 2014.
- P9 M4 workshop, Hamilton, Canada, Dec 2013.
- P8 2013 Symposium on Chemical Physics, Waterloo, Canada, Nov 2013.
- P7 CECAM MCTDH Workshop: High Dimensional Quantum Dynamics: Challenges et opportunities, Birmingham, United Kingdom, Apr 2012.
- P6 Workshop: 4th annual meeting of the COST Action CUSPFEL, Cluj, Romania, Mar 2012.
- P5 CECAM Workshop: New QM/MM opportunities for in silico macromolecular photochemistry, Lyon, France, Feb 2012.
- P4 Satellite of the ninth triennial Congress of the World Association of Theoretical et Computational Chemists: Excited states et non-adiabatic processes in complex systems. Theoretical approaches, San Feliu de Guixols, Spain, Aug 2011.

- P3 Ninth triennial Congress of the World Association of Theoretical et Computational Chemists, Santiago de Compostela, Espagne. **Poster prize:** “An investigation of the photochemical ring-opening of benzopyran”, L. Joubert-Doriol, B. Lasorne, et F. Gatti, Jul 2011.
- P2 Journées dynamiques du sud-ouest, Pau, France, May 2011.
- P1 Rencontre des Chimistes Théoriciens Francophones, Namur, Belgium, Jul 2010.