CV – Benjamin LASORNE

Dr. Benjamin LASORNE

Born 9 March, 1978, in Beauvais (60), France
French citizen

CNRS Research Associate Professor
in Theoretical Chemistry

Institut Charles Gerhardt Montpellier
CTMM
Université de Montpellier
CC 15001, Place Eugène Bataillon
34095 Montpellier, France
Tel: + 33 (0) 4 67 14 36 81
Fax: + 33 (0) 4 67 14 48 39
Email: benjamin.lasorne@univ-montp2.fr

Research Interests

- Theoretical photochemistry

- Non-adiabatic quantum dynamics

- Excited-state quantum chemistry

- Laser control, femtochemistry, attochemistry

Career

- 2013: tenured Research Associate Professor, CNRS, Institut Charles Gerhardt Montpellier, Université Montpellier 2, France

- 2009-2012: tenured Research Assistant Professor, CNRS, Institut Charles Gerhardt Montpellier, Université Montpellier 2, France

- 2004-2008: Post-Doctoral Research Assistant (EPSRC grant), Department of Chemistry, Imperial College London, UK. Group leader: Prof. M. A. Robb

Education

2016: Habilitation in Theoretical Chemistry. Université de Montpellier, France

2004: PhD in Theoretical Chemistry. Université d'Orsay (Paris-Sud 11), France. Supervisor: Prof. M. Desouter-Lecomte

2001: MSc in Molecular Physical Chemistry. ENS Cachan & Université d'Orsay (Paris-Sud 11), France. Supervisor: Prof. M. Desouter-Lecomte

2000: competitive examination for teaching ability in Chemistry. ENS Cachan, France

1998: BSc in Physical Chemistry. Université d'Orsay (Paris-Sud 11), France

1995-1997: two-year highly selective classes to prepare for the competitive examinations to the French Grandes Ecoles, specialised in Physics, Chemistry, and Mathematics, Lycée Clémenceau, Nantes, France

1 Peer-reviewed articles

1. E. Baloitcha, **B. Lasorne**, D. Lauvergnat, G. Dive, Y. Justum, and M. Desouter-Lecomte, "Cumulative reaction probability by constrained dynamics: H transfer in HCN, H_2CO, and H_3CO", J. Chem. Phys. 117 (2002) 727 (DOI: 10.1063/1.1481857)
2. **B. Lasorne**, G. Dive, D. Lauvergnat, and M. Desouter-Lecomte, "Wave packet dynamics along bifurcating reaction paths", J. Chem. Phys. 118 (2003) 5831 (DOI: 10.1063/1.1553978)
3. M.-C. Bacchus-Montabonel, N. Vaeck, **B. Lasorne**, and M. Desouter-Lecomte, "Non-adiabatic effects in the photodissociation of bromoacetyl chloride", Chem. Phys. Lett. 374 (2003) 307 (DOI: 10.1016/S0009-2614(03)00606-7)
4. **B. Lasorne**, M.-C. Bacchus-Montabonel, N. Vaeck, and M. Desouter-Lecomte, "Nonadiabatic interactions in wave packet dynamics of the bromoacetyl chloride photodissociation", J. Chem. Phys. 120 (2004) 1271 (DOI: 10.1063/1.1633759)
5. **B. Lasorne**, F. Gatti, E. Baloitcha, H.-D. Meyer, and M. Desouter-Lecomte, "Cumulative isomerization probability studied by various transition state wave packet methods including the MCTDH algorithm. Benchmark: HCN → CNH isomerization", J. Chem. Phys. 121 (2004) 644 (DOI: 10.1063/1.1760713)
6. **B. Lasorne**, G. Dive, and M. Desouter-Lecomte, "Wave packets in a bifurcating region of an energy landscape: Diels-Alder dimerization of cyclopentadiene", J. Chem. Phys. 122 (2005) 184304 (DOI: 10.1063/1.1891726)
7. **B. Lasorne**, M.-C. Bacchus-Montabonel, N. Vaeck, and M. Desouter-Lecomte, "Quantum dynamics simulations of photodissociation reactions", Int. J. Quant. Chem. 106 (2006) 670 (DOI: 10.1002/qua.20829)
8. **B. Lasorne**, M. J. Bearpark, M. A. Robb, and G. A. Worth, "Direct quantum dynamics using variational multi-configuration Gaussian wavepackets", Chem. Phys. Lett. 432 (2006) 604 (DOI: 10.1016/j.cplett.2006.10.099)
9. **B. Lasorne**, M. A. Robb, and G. A. Worth, "Direct quantum dynamics using variational multi-configuration Gaussian wavepackets. Implementation details and test case", Phys. Chem. Chem. Phys. 9 (2007) 3210 (DOI: 10.1039/b700297a)
10. G. A. Worth, M. A. Robb, and **B. Lasorne**, "Solving the time-dependent Schrödinger equation for nuclear motion in one step: Direct dynamics of non-adiabatic systems", Mol. Phys. 106 (2008) 2077 (DOI: 10.1080/00268970802172503)
11. **B. Lasorne**, F. Sicilia, M. J. Bearpark, M. A. Robb, G. A. Worth, and L. Blancafort, "Automatic generation of active coordinates for quantum dynamics calculations: Application to the dynamics of benzene photochemistry", J. Chem. Phys. 128 (2008) 124307 (DOI: 10.1063/1.2839607)
12. M. Araujo, **B. Lasorne**, M. J. Bearpark, and M. A. Robb, "The photochemistry of formaldehyde: Internal conversion and molecular dissociation in a single step?", J. Phys. Chem. A 112 (2008) 7489 (DOI: 10.1021/jp803152g)
13. **B. Lasorne**, M. J. Bearpark, M. A. Robb, and G. A. Worth, "Controlling S_1/S_0 decay and the balance between photochemistry and photostability in benzene: A direct quantum dynamics study", J. Phys. Chem. A 112 (2008) 13017 (DOI: 10.1021/jp803740a)
14. D. Asturiol, **B. Lasorne**, M. A. Robb, and L. Blancafort, "Photophysics of the π,π^* and n,π^* states of thymine: MS-CASPT2 minimum-energy paths and CASSCF on-the-fly dynamics", J. Phys. Chem. A 113 (2009) 10211 (DOI: 10.1021/jp905303g)
15. M. Araujo, **B. Lasorne**, A. L. Magalhaes, G. A. Worth, M. J. Bearpark, and M. A. Robb, "The molecular dissociation of formaldehyde at medium photoexcitation energies: A quantum chemistry and direct quantum dynamics study", J. Chem. Phys. 131 (2009) 144301 (DOI: 10.1063/1.3242082)
16. D. Asturiol, **B. Lasorne**, G. A. Worth, M. A. Robb, and L. Blancafort, "Exploring the sloped-to-peaked S_2/S_1 seam of intersection of thymine with electronic structure and direct quantum dynamics calculations", Phys. Chem. Chem. Phys. 12 (2010) 4949 (DOI: 10.1039/C001556C)

17. C. S. M. Allan, **B. Lasorne**, G. A. Worth, and M. A. Robb, "A straightforward method of analysis for direct quantum dynamics: Application to the photochemistry of a model cyanine", J. Phys. Chem. A 114 (2010) 8713 (DOI: 10.1021/jp101574b)
18. M. Araujo, **B. Lasorne**, A. L. Magalhaes, M. J. Bearpark, and M. A. Robb, "Controlling product selection in the photodissociation of formaldehyde: Direct quantum dynamics from the S_1 barrier", J. Phys. Chem. A 114 (2010) 12016 (DOI: 10.1021/jp109549r)
19. **B. Lasorne**, M. A. Robb, H.-D. Meyer, and F. Gatti, "The electronic excited states of ethylene with large-amplitude deformations: A dynamical symmetry group investigation", Chem. Phys. 377 (2010) 30 (DOI: 10.1016/j.chemphys.2010.08.011); Erratum, Chem. Phys. 382 (2011) 132 (DOI: 10.1016/j.chemphys.2011.01.004)
20. D. Mendive-Tapia, **B. Lasorne**, G. A. Worth, M. J. Bearpark, and M. A. Robb, "Controlling the mechanism of fulvene S_1/S_0 decay: Switching off the stepwise population transfer", Phys. Chem. Chem. Phys. 12 (2010) 15725 (DOI: 10.1039/c0cp01757d)
21. **B. Lasorne**, G. A. Worth, and M. A. Robb, "Excited-state dynamics", WIREs Comput. Mol. Sci. 1 (2011) 460 (DOI: 10.1002/wcms.26)
22. L. Joubert-Doriol, **B. Lasorne**, F. Gatti, M. Schroder, O. Vendrell, and H.-D. Meyer, "Suitable coordinates for quantum dynamics: Applications using the multiconfiguration time-dependent Hartree (MCTDH) algorithm", Comp. Theor. Chem. 990 (2012) 75 (DOI: 10.1016/j.comptc.2011.12.015)
23. J. Jornet-Somoza, **B. Lasorne**, M. A. Robb, H.-D. Meyer, D. Lauvergnat, and F. Gatti, "A generalised 17-state vibronic-coupling Hamiltonian model for ethylene", J. Chem. Phys. 137 (2012) 084304 (DOI: 10.1063/1.4745861)
24. G. J. Halasz, A. Perveaux, **B. Lasorne**, M. A. Robb, F. Gatti, and A. Vibok, "Simulation of laser-induced quantum dynamics of the electronic and nuclear motion in the ozone molecule on the attosecond time scale", Phys. Rev. A 86 (2012) 043426 (DOI: 10.1103/PhysRevA.86.043426)
25. D. Mendive-Tapia, **B. Lasorne**, G. A. Worth, M. A. Robb, and M. J. Bearpark, "Towards converging non-adiabatic direct dynamics calculations using frozen-width variational Gaussian product basis functions", J. Chem. Phys. 137 (2012) 22A548 (DOI: 10.1063/1.4765087)
26. G. J. Halasz, **A. Perveaux**, B. Lasorne, M. A. Robb, F. Gatti, and A. Vibok, "Coherence revival during the attosecond electronic and nuclear quantum photodynamics of the ozone molecule", Phys. Rev. A 88 (2013) 023425 (DOI: 10.1103/PhysRevA.88.023425)
27. 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 (2014) 044301 (DOI: 10.1063/1.4861226)
28. **B. Lasorne**, J. Jornet-Somoza, H.-D. Meyer, D. Lauvergnat, M. A. Robb, and F. Gatti, "Vertical transition energies vs. absorption maxima, Illustration with the UV absorption spectrum of ethylene", Spectrochim. Acta A Mol. Biomol. Spectrosc. 119 (2014) 52 (DOI: 10.1016/j.saa.2013.04.078)
29. M. Sala, M. Saab, **B. Lasorne**, F. Gatti, and S. Guerin, "Laser control of the radiationless decay in pyrazine using the dynamic Stark effect", J. Chem. Phys. 140 (2014) 194309 (DOI: 10.1063/1.4875736)
30. A. Perveaux, D. Lauvergnat, **B. Lasorne**, F. Gatti, M. A. Robb, G. J. Halasz, and A. Vibok, "Attosecond electronic and nuclear quantum photodynamics of ozone, time-dependent Dyson orbitals and dipole", J. Phys. B 47 (2014) 124010 (DOI: 10.1088/0953-4075/47/12/124010)
31. M. Sala, **B. Lasorne**, F. Gatti, and S. Guerin, "The role of the low-lying dark $n\pi^*$ states in the photophysics of pyrazine, a quantum dynamics study", Phys. Chem. Chem. Phys. 16 (2014) 15957 (DOI: 10.1039/c4cp02165g)
32. **B. Lasorne**, "On the use of Lie group homomorphisms for treating similarity transformations in nonadiabatic photochemistry", Adv. Math. Phys. 2014 (2014) 795730 (DOI: 10.1155/2014/795730)
33. D. Mendive-Tapia, A. Perrier, M. J. Bearpark, M. A. Robb, **B. Lasorne**, and D. Jacquemin, "New insights into the by-product fatigue mechanism of the photo-induced ring-opening in diarylethenes", Phys. Chem. Chem. Phys. 16 (2014) 18463 (DOI: 10.1039/C4CP03001J)

34. M. Saab, L. Joubert Doriol, **B. Lasorne**, S. Guerin, and F. Gatti, "A quantum dynamics study of the benzopyran ring opening guided by laser pulses", Chem. Phys. 442 (2014) 93 (DOI: 10.1016/j.chemphys.2014.01.016)
35. A. Perveaux, D. Lauvergnat, F. Gatti, G. J. Halasz, A. Vibok, and **B. Lasorne**, "Monitoring the birth of an electronic wavepacket in a molecule with attosecond time-resolved photoelectron spectroscopy", J. Phys. Chem. A 118 (2014) 8773 (DOI: 10.1021/jp508218n)
36. M. Saab, M. Sala, **B. Lasorne**, F. Gatti, and S. Guerin, "Full-dimensional control of the radiationless decay in pyrazine using the dynamic Stark effect", J. Chem. Phys. 141 (2014) 134114 (DOI: 10.1063/1.4896938)
37. A. Perveaux, P. J. Castro, D. Lauvergnat, M. Reguero, and **B. Lasorne**, "Intramolecular charge transfer in 4-aminobenzonitrile does not need the twist and may not need the bend", J. Phys. Chem. Lett. 6 (2015) 1316 (DOI: 10.1021/acs.jpclett.5b00162)
38. G. W. Richings, I. Polyak, K. E. Spinlove, G. A. Worth, I. Burghardt, and **B. Lasorne**, "Quantum dynamics simulations using Gaussian wavepackets: The vMCG method", Int. Rev. Phys. Chem. 34 (2015) 269 (DOI: 10.1080/0144235X.2015.1051354)
39. **B. Lasorne**, A. Fihey, D. Mendive-Tapia, and D. Jacquemin, "A curve-crossing model to rationalize and optimize diarylethene dyads", Chem. Sci. 6 (2015) 5695 (DOI: 10.1039/C5SC01960E)
40. D. Mendive-Tapia, L. Kortekaas, J. D. Steen, A. Perrier, **B. Lasorne**, W. R. Browne, and D. Jacquemin, "Accidental degeneracy in the spiropyran radical cation: Charge transfer between two orthogonal rings inducing ultra-efficient reactivity", Phys. Chem. Chem. Phys. 18 (2016) 31244 (DOI: 10.1039/C6CP06907J)
41. P. Decleva, N. Quadri, A. Perveaux, D. Lauvergnat, F. Gatti, **B. Lasorne**, G. J. Halasz, and A. Vibok, "Attosecond electronic and nuclear quantum photodynamics of ozone monitored with time and angle resolved photoelectron spectra", Sci. Rep. 6 (2016) 36613 (DOI: 10.1038/srep36613)
42. A. Perveaux, M. Lorphelin, **B. Lasorne**, and D. Lauvergnat, "Fast and slow excited-state intramolecular proton transfer in 3-hydroxychromone: A two-state story?", Phys. Chem. Chem. Phys. 19 (2017) 6579 (DOI: 10.1039/C6CP06603H)
43. E. K.-L. Ho, T. Etienne, and **B. Lasorne**, "Vibronic properties of para -polyphenylene ethynylenes: TD-DFT insights", J. Chem. Phys. 146 (2017) 164303 (DOI: 10.1063/1.4981802)
44. B. Gonon, A. Perveaux, F. Gatti, D. Lauvergnat, and **B. Lasorne**, "On the applicability of a wavefunction-free, energy-based procedure for generating first-order non-adiabatic couplings around conical intersections", J. Chem. Phys. 147 (2017) 114114 (DOI: 10.1063/1.4991635)
45. A. Perveaux, P. J. Castro, D. Lauvergnat, M. Reguero, and **B. Lasorne**, "Ultrafast internal conversion in 4-aminobenzonitrile occurs sequentially along the seam", Chem. Phys. (2018) in press [DOI: 10.1016/j.chemphys.2018.03.013]

2 Proceedings

1. G. J. Halasz, A. Perveaux, **B. Lasorne**, M. A. Robb, F. Gatti, and A. Vibok, "Attosecond electronic and nuclear quantum photodynamics of the ozone molecule", AIP Conf. Proc. 1565 (2013) 19 (DOI: 10.1063/1.4833688)
2. A. Perveaux, P. J. Castro, M. Reguero, H.-D. Meyer, F. Gatti, **B. Lasorne**, and D. Lauvergnat, "Multidimensional photochemistry model: Application to aminobenzonitrile and benzopyran", Springer Proc. Phys. 162 (2015) 386 (DOI: 10.1007/978-3-319-13242-6_94)

3 Edited-book chapters

1. **B. Lasorne**, M. J. Bearpark, M. A. Robb, and G. A. Worth, "Quantum direct dynamics applied to the intelligent control of benzene photochemistry", in: Coherent Control of Molecules, B. Lasorne and G. A. Worth (Eds.) p. 34 (CCP6, Daresbury, 2006) (ISBN: 0-9545289-5-6)
2. **B. Lasorne** and G. A. Worth, "Direct dynamics with quantum nuclei", in: Multidimensional Quantum Dynamics: MCTDH Theory and Applications, H.-D. Meyer, F. Gatti, and G. A. Worth (Eds.), (Wiley-VCH, Weinheim, 2009) p. 113 (DOI: 10.1002/9783527627400.ch13; ISBN: 9783527320189)
3. L. Blancafort, **B. Lasorne**, M. J. Bearpark, G. A. Worth, and M. A. Robb, "Second-order analysis of conical intersections: Applications to photochemistry and photophysics of organic molecules", in: The Jahn-Teller Effect – Fundamentals and Implications for Physics and Chemistry, H. Köppel, D. R. Yarkony, and H. Barentzen (Eds.), Springer Series in Chemical Physics, Vol. 97, (Springer, Heidelberg, 2009) p. 169 (ISBN: 978-3-642-03431-2)
4. F. Gatti and **B. Lasorne**, "Introduction and conceptual background"; "Conclusions", in: Molecular Quantum Dynamics – From Theory to Applications, F. Gatti (Ed.), Physical Chemistry in Action, (Springer, Heidelberg, 2014) p. 1; p. 271 (ISBN: 978-3-642-45289-5)
5. **B. Lasorne**, G. A. Worth, and M. A. Robb. "Non-adiabatic photochemistry: Ultrafast electronic state transitions and nuclear wavepacket coherence", in: Molecular Quantum Dynamics – From Theory to Applications, F. Gatti (Ed.), Physical Chemistry in Action (Springer, Heidelberg, 2014) p. 181 (ISBN: 978-3-642-45289-5)

4 Edited book

1. B. Lasorne and G. A. Worth, Coherent Control of Molecules (CCP6, Daresbury, 2006) ISBN: 0-9545289-5-6

5 Book

1. F. Gatti, B. Lasorne, H.-D. Meyer, and A. Nauts, Applications of Quantum Dynamics in Chemistry, Lectures Notes in Chemistry (Springer International Publishing, Cham, 2017) (ISBN: 978-3-319-53923-2 & 978-3-319-53921-8) (DOI: 10.1007/978-3-319-53923-2)

6 Invited talks

6.1 International audience

1. B. Lasorne, M. A. Robb, G. A. Worth, "Interfacing MCTDH to ab initio codes". QDFrame: Providing a Framework for Quantum Dynamics Simulation Codes, Birmingham, United Kingdom, 14-15 December 2009
2. B. Lasorne, M. A. Robb, H.-D. Meyer, F. Gatti, "The electronic excited states of ethylene with large-amplitude deformations: A dynamical symmetry group investigation", XXth International Symposium on the Jahn-Teller Effect: Where Are the Nuclei Going – in Response of What the Electrons Are Doing?, Fribourg, Switzerland, 16-20 August 2010
3. B. Lasorne, M. A. Robb, H.-D. Meyer, F. Gatti, "The electronic excited states of ethylene with large-amplitude deformations: A dynamical symmetry group investigation", 3rd Annual Workshop of the COST Action CM0702 – Chemistry with Ultrashort Pulses and Free-Electron Lasers: Looking for Control Strategies through "Exact" Computations (CUSPFEL), Hersonissos, Greece, 20-22 October 2010
4. B. Lasorne, M. Araujo, C. S. M. Allan, M. J. Bearpark, G. A. Worth, M. A. Robb, "The direct dynamics variational multiconfiguration Gaussian wavepacket method. Application to photochemical reactions",

CECAM Meeting – Adiabatic and Non-Adiabatic Methods in Quantum Dynamics, Lausanne, Switzerland, 1-3 November 2010

5. B. Lasorne, M. A. Robb, H.-D. Meyer, F. Gatti, "The electronic excited states of ethylene and large-amplitude deformations: A dynamical symmetry group investigation", ACS Fall 2011 National Meeting & Exposition, Denver, Colorado, United States, 28 August-1 September 2011
6. B. Lasorne, J. Jornet-Somoza, M. A. Robb, H.-D. Meyer, D. Lauvergnat, F. Gatti, "A generalised 17-state vibronic-coupling Hamiltonian model for ethylene", Conference on Theory and Applications of Computational Chemistry 2012 (TACC-2012), Pavia, Italy, 2-7 September 2012
7. B. Lasorne, F. Gatti, A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, D. Lauvergnat, H.-D. Meyer, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, "Diabatic strategies for photochemical quantum dynamics", XLIC Working Group 3: Control of Chemical Reactivity 2014, Birmingham, United Kingdom, 14-16 April 2014
8. B. Lasorne, F. Gatti, A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, D. Lauvergnat, H.-D. Meyer, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, "Diabatic strategies for photochemical quantum dynamics", CECAM Meeting – Recent progress in adiabatic and non-adiabatic methods in quantum dynamics, Lausanne, Switzerland, 12-15 May 2014
9. M. Araujo, C. S. M. Allan, D. Mendive-Tapia, M. J. Bearpark, G. A. Worth, M. A. Robb, B. Lasorne, "Gaussian-based direct quantum dynamics applied to non-adiabatic photochemistry", Current Topics in Theoretical Chemistry (CTTC2014), Nha Trang, Vietnam, 25-29 August 2014
10. A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, F. Gatti, D. Lauvergnat, H.-D. Meyer, P. J. Castro, M. Reguero, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, B. Lasorne, "Diabatic strategies for photochemical quantum dynamics", 15th Chinase-French Workshop in Theoretical Chemistry (CFWTC 2015), Strasbourg, France, 10-13 May 2015
11. A. Perveaux, D. Lauvergnat, F. Gatti, A. Toth, G. J. Halasz, A. Vibok, B. Lasorne, "Monitoring coherences in neutral molecules on the subfemtosecond timescale", 3rd XLIC General Meeting (COST Action CM1204 – XUV/X-Ray Light and Fast Ions for Ultrafast Chemistry), Debrecen, Hungary, 2-4 November 2015
12. A. Perveaux, F. Gatti, D. Lauvergnat, H.-D. Meyer, P. J. Castro, M. Reguero, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, B. Lasorne, "Diabatic strategies for photochemical quantum dynamics", 2nd XLIC WG1 Meeting, Ultrafast electron dynamics in molecules (COST Action CM1204 – XUV/X-Ray Light and Fast Ions for Ultrafast Chemistry), Edinburgh, United Kingdom, 29-30 August 2016
13. B. Lasorne, A. Perveaux, D. Mendive-Tapia, E. Ho, M. Lorphelin, M.-L. Doublet, T. Etienne, D. Lauvergnat, M. A. Robb, M. J. Bearpark, G. A. Worth, "Diabatic strategies for molecular and macromolecular photodynamics", ESBS 2016 Workshop (Excited States Simulations: Bridging Scales), Marseille, France, 7-10 November 2016
14. M. Araujo, C. S. M. Allan, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, B. Lasorne, "Gaussian-based direct quantum dynamics applied to non-adiabatic photochemistry", 5th Molcas Developers' Workshop, Jerusalem, Israel, 7-10 February 2017
15. B. Lasorne, M. Araujo, C. S. M. Allan, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, "Direct dynamics with vMCG: applications to ultrafast photochemistry and control", Quantum Dynamics with the MCTDH Method: Future and Perspectives, Orsay, France, 25 September-20 October 2017

6.2 National audience

1. B. Lasorne, A. Perveaux, D. Mendive-Tapia, M. Lorphelin, D. Lauvergnat, M. A. Robb, M. J. Bearpark, G. A. Worth, "Quantum dynamics applied to ultrafast phenomena", Deuxième réunion plénière du GDR Ultrafast Phenomena, Paris, France, 9-10 November 2017

7 Contributed talks

7.1 International audience

1. B. Lasorne, M. Desouter-Lecomte, G. Dive, M.-C. Bacchus-Montabonel, N. Vaeck, “Dynamique quantique dans des régions critiques des surfaces de potentiel”. 9ème Rencontre des Chimistes Théoriciens Français, Pau, France, 20-24 September 2004
2. B. Lasorne, M. J. Bearpark, M. A. Robb, G. A. Worth, “Direct dynamics using variational Gaussian wavepackets. Application to NOCl photodissociation and benzene non-adiabatic photochemistry”. Collaborative Computational Project on Molecular Quantum Dynamics (CCP6) – Workshop on Coherent Control of Molecules, Birmingham, United Kingdom, 3-5 July 2006
3. B. Lasorne, M. J. Bearpark, M. A. Robb, G. A. Worth, “Dynamique quantique ‘on-the-fly’ appliquée à l’étude de systèmes photochimiques”. 10ème Rencontre des Chimistes Théoriciens Francophones, Nancy, France, 10-13 July 2006
4. B. Lasorne, M. J. Bearpark, M. A. Robb, G. A. Worth, “Direct dynamics using variational Gaussian wavepackets. Application to the intelligent control of benzene photochemistry”. 2007 American Physical Society March Meeting (Focus Session: Non-adiabatic Molecular Dynamics and Control at Conical Intersections), Denver, Colorado, United States, 5-9 March 2007
5. Lasorne, F. Sicilia, G. A. Worth, M. J. Bearpark, L. Blancafort, M. A. Robb, “Direct quantum dynamics using variational Gaussian wavepackets. Application to laser-driven control of benzene photochemistry”. 2nd Workshop on High Dimensional quantum dynamics: challenges and opportunities, La Grande Motte, France, 25-28 February 2008
6. B. Lasorne, M. Araujo, F. Sicilia, G. A. Worth, M. J. Bearpark, L. Blancafort, M. A. Robb, “Controlling photochemistry: dynamical pathways leading to seams of conical intersection”. XIX International Symposium on the Jahn-Teller Effect: Vibronic Interactions and Orbital Physics in Molecules and in the Condensed Phase, Heidelberg, Germany, 25-29 August 2008
7. B. Lasorne, M. A. Robb, H.-D. Meyer, F. Gatti, “Etats électroniques excités de l’éthylène et mouvements de grande amplitude : description dans le groupe de symétrie dynamique”, 12ème Rencontre des Chimistes Théoriciens Francophones, Namur, Belgium, 4-8 July 2010
8. B. Lasorne, M. A. Robb, H.-D. Meyer, F. Gatti, “The electronic excited states of ethylene and large-amplitude deformations: A dynamical symmetry group investigation”, Excited States and Non-Adiabatic Processes in Complex Systems. Theoretical Approaches. Satellite of the WATOC 2011», Sant Feliu de Guíxols, Spain, 25-27 July 2011
9. B. Lasorne, M. Araujo, C. S. M. Allan, D. Mendive-Tapia, M. J. Bearpark, G. A. Worth, M. A. Robb, “The direct dynamics variational multiconfiguration Gaussian wavepacket method. Application to photochemistry and photophysics”, High-Dimensional Quantum Dynamics: Challenges and Opportunities 2012 (HDQD 2012), Birmingham, United Kingdom, 12-14 April 2012
10. B. Lasorne, A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, F. Gatti, D. Lauvergnat, H.-D. Meyer, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, “Diabatic strategies for photochemical quantum dynamics”, High-Dimensional Quantum Dynamics: Challenges and Opportunities (HDQD 2014), Mittelwihr, France, 2-6 September 2014
11. B. Lasorne, M. Araujo, C. S. M. Allan, D. Mendive-Tapia, M. J. Bearpark, G. A. Worth, M. A. Robb, “Gaussian-based direct quantum dynamics applied to non-adiabatic photochemistry”, MPM Conference (Modeling Photoactive Molecules), Nantes, France, 21-24 April 2015
12. A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, F. Gatti, D. Lauvergnat, H.-D. Meyer, P. J. Castro, M. Reguero, B. Lasorne, “Diabatic strategies for photochemical quantum dynamics”, The Chemical Bonds at the 21st Century (a satellite of ICQC, 2015), Xiamen, China, 14-18 June 2015
13. B. Lasorne, A. Fihey, D. Mendive-Tapia, A. Perveaux, P. J. Castro, D. Lauvergnat, D. Jacquemin. M. Reguero, “Multiphotochromism and dual fluorescence: theoretical models and computations”, MRP Conference (Multi-Responsive Photochromes), Nantes, France, 25-28 April 2016

14. B. Lasorne, A. Perveaux, D. Mendive-Tapia, M. Lorphelin, D. Lauvergnat, M. A. Robb, M. J. Bearpark, G. A. Worth, “Diabatic strategies for molecular photodynamics”, XLIII Congress of Theoretical Chemists of Latin Expression (CHITEL 2017), Paris, France, 3-7 July 2017

7.2 National audience

1. B. Lasorne, A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, F. Gatti, D. Lauvergnat, H.-D. Meyer, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, “Stratégies diabatiques pour la dynamique quantique photochimique”, 2ème congrès annuel du GDR ThéMS, Bordeaux, France, 9-10 December 2014
2. A. Perveaux, L. Joubert-Doriol, J. Jornet-Somoza, F. Gatti, D. Lauvergnat, H.-D. Meyer, P. J. Castro, M. Reguero, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, B. Lasorne, “Diabatic strategies for photochemical quantum dynamics”, Journées Dynamiques du Sud-Ouest 2015 (JDSO 2015), Toulouse, France, 4-5 June 2015

8 Posters

8.1 International audience

1. B. Lasorne, M. Desouter-Lecomte, E. Baloitcha, D. Lauvergnat, Y. Justum, N. Vaeck, M.-C. Bacchus-Montabonel, G. Dive, “Dynamics around critical points of the PES with constrained Hamiltonians”. 37. Symposium für Theoretische Chemie. Electronically Excited Molecules: Structure and Dynamics, Bad Herrenalb, Germany, 23-27 September 2001
2. B. Lasorne, M. Desouter-Lecomte, E. Baloitcha, D. Lauvergnat, G. Dive, N. Vaek, M.-C. Bacchus-Montabonel, “Dynamics around critical points of the PES with constrained Hamiltonians”. Quantum Chemistry in Belgium: Vth meeting, Liège, Belgium, 16 November 2001
3. B. Lasorne, M. Desouter-Lecomte, E. Baloitcha, D. Lauvergnat, G. Dive, N. Vaeck, M.-C. Bacchus-Montabonel, “Dynamique autour de points critiques des surfaces d’énergie potentielle par la méthode des hamiltoniens contraints”. 8ème Rencontre des Chimistes Théoriciens Francophones, Strasbourg, France, 16-20 September 2002
4. B. Lasorne, M. Desouter-Lecomte, E. Baloitcha, D. Lauvergnat, G. Dive, N. Vaeck, M.-C. Bacchus-Montabonel, “Dynamics around critical points of the PES with constrained Hamiltonians”. Quantum Dynamical Concepts: From Diatomics to Biomolecules, Seminar and Workshop, Dresden, Germany, 2 April-5 May 2002
5. B. Lasorne, M. Desouter-Lecomte, D. Lauvergnat, G. Dive, “Quantum dynamics in reduced dimensionality”. XVIII International Conference on Molecular Energy Transfer, San Lorenzo de El Escorial, Spain, 15-20 June 2003
6. M. Desouter-Lecomte, B. Lasorne, M.-C. Bacchus-Montabonel, N. Vaeck, “Wave packet simulation of the nonadiabatic competitive dissociation of excited bromoacetyl chloride”. XVIII International Conference on Molecular Energy Transfer, San Lorenzo de El Escorial, Spain, 15-20 June 2003
7. B. Lasorne, M. Desouter-Lecomte, G. Dive, M.-C. Bacchus-Montabonel, N. Vaeck, E. Baloïtcha, F. Gatti, H.-D. Meyer, “Reactivity by Wave Packet Dynamics in Reduced Dimensionality”. Modelling and Understanding in Theoretical Chemistry, a Conference in Honour of Jacopo Tomasi, Lucca, Italy, 1-4 August 2004
8. B. Lasorne, M. J. Bearpark, M. A. Robb, G. A. Worth, “Direct dynamics using variational Gaussian wavepackets. Application to NOCl photodissociation and benzene non-adiabatic photochemistry”. International Symposium on the Jahn-Teller Effect: Novel Aspects in Orbital Physics and Vibronic Dynamics of Molecules and Crystals, Trieste, Italy, 28-31 August 2006

9. B. Lasorne, F. Sicilia, G. A. Worth, M. J. Bearpark, L. Blancafort, M. A. Robb, "Controlling photochemistry: dynamical pathways leading to seams of conical intersection", XIIIth International Congress of Quantum Chemistry, Helsinki, Finland, 22-27 June 2009
10. B. Lasorne, J. Jornet-Somoza, M. A. Robb, H.-D. Meyer, F. Gatti "The electronic excited states of ethylene and large-amplitude deformations: A dynamical symmetry group investigation", 2011 World Congress of the World Association of Theoretical and Computational Chemists (WATOC 2011), Santiago de Compostela, Spain, 17-22 July 2011
11. B. Lasorne, M. Araujo, C. S. M. Allan, D. Mendive-Tapia, M. J. Bearpark, G. A. Worth, M. A. Robb, "The direct dynamics variational multiconfiguration Gaussian wavepacket method. Application to photochemistry and photophysics", Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics (satellite symposium of the 14th International Congress of Quantum Chemistry, ICQC 2012), Minneapolis, Minnesota, United States, 20-22 June 2012
12. G. J. Halasz, A. Perveaux, B. Lasorne, M. A. Robb, F. Gatti, A. Vibok, "Simulation of laser-induced quantum dynamics of the electronic and nuclear motion in the ozone molecule on the attosecond time scale", 4th International Conference on Attosecond Physics (ATTO2013), Paris, France, 8-10 July 2013
13. J. Jornet-Somoza, L. Joubert Doriol, A. Perveaux, D. Lauvergnat, H.-D. Meyer, M. A. Robb, F. Gatti, B. Lasorne, "Strategies for photochemical quantum dynamics", Excited States and Complex Environments (ESCE-2013), Münster, Germany, 8-11 October 2013
14. A. Perveaux, F. Gatti, D. Lauvergnat, H.-D. Meyer, P. J. Castro, M. Reguero, D. Mendive-Tapia, M. A. Robb, M. J. Bearpark, G. A. Worth, B. Lasorne, "Diabatic strategies for photochemical quantum dynamics", Ultrafast Imaging of Photochemical Dynamics: Faraday Discussion, Edinburgh, United Kingdom, 31 August-2 September 2016
15. B. Lasorne, A. Perveaux, D. Mendive-Tapia, E. K.-L. Ho, M. Lorphelin, M.-L. Doublet, T. Etienne, D. Lauvergnat, M. A. Robb, M. J. Bearpark, G. A. Worth, "Diabatic strategies for molecular and macromolecular photodynamics", 28th International Conference on Photochemistry (ICP 2017), Strasbourg, France, 16-21 July 2017

8.2 National audience

1. B. Lasorne, F. Sicilia, G. A. Worth, M. J. Bearpark, L. Blancafort, M. A. Robb, "Controlling photochemistry: dynamical pathways leading to seams of conical intersection", 3èmes Journées de Dynamique du Sud-Ouest (JDSO 2009), Bordeaux, France, 27-28 May 2009
2. A. Perveaux, G. J. Halasz, B. Lasorne, M. A. Robb, F. Gatti, A. Vibok, "Laser-induced dynamics simulations of the electronic and nuclear motions in ozone on the attosecond time scale", 5èmes Journées de Dynamique du Sud-Ouest (JDSO 2013), Perpignan, France, 4-5 June 2013

9 Seminars

1. "Quantum dynamics in reduced dimensionality", Institut für Physikalische Chemie, Kiel, Germany, 9 July 2003
2. "Réactivité dans des régions critiques des surfaces de potentiel. Traitement quantique en dimension réduite", Laboratoire de Laboratoire de Spectrométrie Ionique et Moléculaire, Lyon, France, 18 March 2004
3. "Réactivité dans des régions critiques des surfaces de potentiel. Traitement quantique en dimension réduite", Laboratoire de Chimie Physique, Orsay, France, 26 March 2004
4. "Dynamique quantique 'on-the-fly' appliquée à l'étude de systèmes photochimiques", Laboratoire de Structure et Dynamique des Systèmes Moléculaires et Solides, Montpellier, France, 26 June 2006

5. “Dynamique quantique ‘on-the-fly’ appliquée au contrôle cohérent de la photochimie du benzène”, Laboratoire de Structure et Dynamique des Systèmes Moléculaires et Solides, Montpellier, France, 27 November 2006
6. “Dynamique quantique ‘on-the-fly’ appliquée à l’étude de systèmes photochimiques”, Laboratoire de Chimie Physique, Orsay, France, 7 January 2008
7. “Direct quantum dynamics applied to photochemistry”, Departamento de Química, Universidade do Porto, Porto, Portugal, 30 October 2009
8. “Etats électroniques excités de l’éthylène et déformations de grande amplitude : description dans le groupe de symétrie dynamique”, Laboratoire de Chimie Quantique, Université de Strasbourg, Strasbourg, France, 20 January 2012
9. “The direct dynamics variational multiconfiguration Gaussian wavepacket method. Application to photophysics and photochemistry”, Nano-Bio Spectroscopy Group / European Theoretical Spectroscopy Facility, Centro Joxe Mari Korta, Donostia-San Sebastian, Spain, 16 September 2013
10. “Diabatic Strategies for Photochemical Quantum Dynamics”, Quantum Chemistry Group, Universitat Rovira i Virgili, Tarragona, Spain, 23 April 2014
11. “Diabatic strategies for photochemical quantum dynamics”, Laboratoire de Chimie et de Physique Quantiques, Université Paul Sabatier, Toulouse, France, 2 October 2014
12. “Phénomènes photo-induits : de la molécule aux architectures complexes”, Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, Paris, France, 11 July 2016
13. “Theoretical Photochemistry: Concepts, Formalisms, Examples”, Department of Chemistry, Xiamen University, Xiamen, China, 22 et 23 November 2016
14. “Diabatic Strategies for Molecular Photodynamics”, Department of Chemistry, Xiamen University, Xiamen, China, 27 April 2018