Publication List

Mario Barbatti

List compiled on January 27, 2015.

See updated information at www.barbatti.org/publication

Contents

Bibliometric Indicators

- Peer-reviewed papers: 101 (1999-2015; corresponding author in 65)
- Book chapters: 6 (2005-2014)
- Full articles in proceedings: 3
- Manuals, white papers, and other publications: 4
- Editorial works: 3
- Number of citations: 2898
- H-index: 31 i-10 index: 77
- Google Scholar profile: tiny.cc/gscholar Research ID: F-5647-2014

Peer-reviewed Papers

1. T. M. Cardozo, A. J. A. Aquino, **M. Barbatti**, I. Borges Jr., and H. Lischka, **Absorption and Fluorescence Spectra of Poly-(p-phenylene vinylene) (PPV) oligomers: An Ab Initio Simulation**, J. Phys. Chem. A, doi:10.1021/jp508512s (2014).
   doi:10.1021/jp508512s
2. G. P. Rodrigues E. Ventura, S. do Monte, **M. Barbatti**, **Photochemical Deactivation Process of HCFC-133a ($C_2H_2F_3Cl$): A Nonadiabatic Dynamics Study**; J. Phys. Chem. A **118**, 12041 (2014).
   doi:10.1021/jp507681g
3. A. Luzio, D. Fazzi, F. Nübling, R. Matsidik, A. Straub, H. Komber, E. Giussani, S. Watkins, **M. Barbatti**, W. Thiel, E. Gann, L. Thomsen, C. McNeill, M. Caironi, M. Sommer, **Structure-function relationships of high-electron mobility naphthalene diimide copolymers prepared by direct arylation**; Chem. Mater. **26**, 6233 (2014).
   doi:10.1021/cm503033j
4. **M. Barbatti**, **Photorelaxation induced by water-chromophore electron transfer**; J. Am. Chem. Soc. **136**, 10246 (2014).
   doi:10.1021/ja505387c
5. **M. Barbatti**, **Computational reference data for photochemistry of cyclobutane pyrimidine dimers**; ChemPhysChem **15**, 3342 (2014).
   doi:10.1002/cphc.201402302
6. I. Antol, Z. Glasovac, R. Crespo-Otero, M. Barbatti, **Guanidine and guanidinium cation in the excited state – theoretical investigation**; J. Chem. Phys. **141**, 074307 (2014).
   doi:10.1063/1.4892569

7. R. Crespo-Otero, A. Mardykov, E. Sanchez-Garcia, W. Sander, M. Barbatti, **Photo-stability of peptide-bond aggregates: N-methylformamide dimers**; Phys. Chem. Chem. Phys. **16**, 18877 (2014). doi:10.1039/C4CP02518K

8. F. Plasser, R. Crespo-Otero, M. Pederzoli, J. Pittner, H. Lischka, **M. Barbatti**, **Surface hopping dynamics with correlated single-reference methods: 9H-adenine as a case study**; J. Chem. Theory Comput. **10**, 1395 (2014). doi:10.1021/ct4011079

9. N. Kungwan, K. Kerdpol, R. Daengngern, S. Hannongbua, **M. Barbatti**, **Effects of the second hydration shell on excited-state multiple proton transfer: Dynamics simulations of 7-azaindole:$(H_2O)_{1-5}$ clusters in the gas phase**; Theor. Chem. Acc. **133**, 1480 (2014). doi:10.1007/s00214-014-1480-y

10. A. C. West, **M. Barbatti**, H. Lischka, T. L. Windus, **Nonadiabatic dynamics study of methaniminium with ORMAS: Challenges of incomplete active spaces in dynamics simulations**; Comput. Theor. Chem. **1040-1041**, 158 (2014). doi:10.1016/j.comptc.2014.03.015

11. K. Sen, R. Crespo-Otero, W. Thiel, **M. Barbatti**, **Electronic structure of fullerene-squaraine complexes for photovoltaic devices**; Comput. Theor. Chem. **1040-1041**, 237 (2014). doi:10.1016/j.comptc.2014.02.024

12. **M. Barbatti**, M. Ruckenbauer, F. Plasser, J. Pittner, G. Granucci, M. Persico, H. Lischka **NEWTON-X: a surface-hopping program for nonadiabatic molecular dynamics**; WIREs: Comp. Mol. Sci. 4, 26 (2014). doi:10.1002/wcms.1158

13. E. Boulanger, A. Anoop, D. Nachtigallova, W. Thiel, **M. Barbatti**, **Photochemical Steps in Prebiotic Synthesis of Purine Precursors from HCN**; Angew. Chem. Int. Ed. **52**, 8000 (2013). doi:10.1002/anie.201303246

14. D. Asturiol, **M. Barbatti**, **Electronic states of porphycene-O_2 complex and photoinduced singlet O_2 production**; J. Chem. Phys. **139**, 074307 (2013). doi:10.1063/1.4818490

15. N. Kungwan, R. Daengngern, T. Piansawan, S. Hannongbua, **M. Barbatti**, **Theoretical study on excited-state intermolecular proton transfer reactions of 1H-pyrrolo[3,2-h]quinoline with water and methanol**; Theor. Chem. Acc. **132**, 1397 (2013). doi:10.1007/s00214-013-1397-x

16. R. Daengngern, K. Kerdpol, N. Kungwan, S. Hannongbua, **M. Barbatti**, **Dynamics simulations of excited-state triple proton transfer in 7-azaindole complexes with water, water-methanol and methanol**; J. Photochem. Photobiol. A **266**, 28 (2013). doi:10.1016/j.jphotochem.2013.05.012

17. B. Sellner, **M. Barbatti**, T. Müller, W. Domcked, H. Lischka, **Ultrafast Nonadiabatic Dynamics of Ethylene Including Rydberg States**; Mol. Phys. **111**, 2439 (2013). doi:10.1080/00268976.2013.813590

18. M. Ruckenbauer, **M. Barbatti**, T. Müller, H. Lischka**, Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment**; J. Phys. Chem. A **117**, 2790 (2013). doi:10.1021/jp400401f

19. K. Sen, R. Crespo-Otero, O. Weingart, W. Thiel, **M. Barbatti, Interfacial states in donor-acceptor organic heterojunctions: computational insights into thiophene-oligomer/fullerene junctions**; J. Chem. Theory Comput. **9**, 533 (2013). doi:10.1021/ct300844y

20. R. Crespo-Otero, A. Mardyukov, E. Sanchez-Garcia, **M. Barbatti**, W. Sander, **Photochemistry of N-Methylformamide: Matrix Isolation and Nonadiabatics Dynamics**; ChemPhysChem. **14**, 827 (2013). doi:10.1002/cphc.201200573

21. M. G. P. Homem, A. Lopez-Castillo, **M. Barbatti**, L. F. S. Rosa, P. Iza, R. L. Cavasso-Filho, L. S. Farenzena, M. T. Lee, I. Iga, **Experimental and theoretical investigations on photoabsorption and photoionization of trimethylphosphate in the vacuum-ultraviolet energy range**; J. Chem. Phys. **137**, 184305 (2012). doi:10.1063/1.4765336

22. F. Plasser, G. Granucci, J. Pittner, **M. Barbatti**, M. Persico, H. Lischka, **Surface hopping dynamics using a locally diabatic formalism: charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer**; J. Chem. Phys. **137**, 22A314 (2012). doi:10.1063/1.4738960

23. **M. Barbatti**, Z. Lan, R. Crespo-Otero, J. J. Szymczak, H. Lischka, and W. Thiel, **Critical appraisal of excited-state nonadiabatic dynamics simulations of 9H-adenine**; J. Chem. Phys. **137**, 22A503 (2012). doi:10.1063/1.4731649

24. R. Crespo-Otero and **M. Barbatti**, **Spectrum simulation and decomposition with nuclear ensemble: formal derivation and application to benzene, furan and 2-phenylfuran**; Theor. Chem. Acc. **131**, 1237 (2012). doi:10.1007/s00214-012-1237-4

25. N. Kungwan, F. Plasser, A. J. A. Aquino, **M. Barbatti**, P. Wolschann, and Hans Lischka, **The effect of Hydrogen Bonding on the Excited-State Proton Transfer in 2,(2'-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study**; Phys. Chem. Chem. Phys. **14**, 9016 (2012). doi:10.1039/C2CP23905A

26. Z. Lan, S. Nonell, and **M. Barbatti**, **Theoretical Characterization of Absorption and Emission Spectra of an Asymmetric Porphycene**; J. Phys. Chem. A **116**, 3366 (2012). doi:10.1021/jp300888a

27. **M. Barbatti** and M. A. C. Nascimento, **Does the H_5^+ hydrogen cluster exist in dense interstellar clouds?**; Int. J. Quantum Chem. **112**, 3169 (2012). doi:10.1002/qua.24110

28. F. Plasser, **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **Electronically excited states and photodynamics: a continuing challenge**; Theor. Chem. Acc. **131**, 1073 (2012). doi:10.1007/s00214-011-1073-y

29. R. Daengngern, N. Kungwan, P. Wolschann, A. J. A. Aquino, H. Lischka, and **M. Barbatti**, **Excited-State Intermolecular Proton Transfer Reactions of 7-Azaindole(MeOH)$_n$ (n=1-3) Clusters in the Gas Phase: On-the-fly Dynamics Simulation**; J. Phys. Chem. A **115**, 14129 (2011). doi:10.1021/jp2059936

30. R. Crespo-Otero, **M. Barbatti**, H. Yu, N. L. Evans, and S. Ullrich, **The ultrafast dynamics of UV-excited imidazole**; ChemPhysChem. **12**, 3365 (2011). doi:10.1002/cphc.201100453

31. **M. Barbatti** and S. Ullrich, **Ionization potentials of adenine along the internal conversion pathways**; Phys. Chem. Chem. Phys. **13**, 15492 (2011). dx.doi.org/10.1039/C1CP21350D

32. M. Pederzoli, J. Pittner, **M. Barbatti**, and H. Lischka, **A non-adiabatic molecular dynamics study of the cis - trans isomerization of azobenzene excited to the S_1 state**; J. Phys. Chem. A **115**, 11136 (2011). dx.doi.org/10.1021/jp2013094

33. I. Borges Jr., **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **Electronic spectra of nitroethylene**; Int. J. Quantum. Chem. **112**, 1225 (2012). doi:10.1002/qua.23080

34. D. Nachtigallova, A. J. A. Aquino, J. J Szymczak, **M. Barbatti**, P. Hobza, and H. Lischka, **Non-Adiabatic Dynamics of Uracil: Population Split Among Different Decay Mechanisms**; J. Phys. Chem. A **115**, 5247 (2011). doi:10.1021/jp201327w

35. R. Crespo-Otero and **M. Barbatti**, **$Cr(CO)_6$ photochemistry: Semi-classical study of UV absorption spectral intensities and dynamics of photodissociation**; J. Chem. Phys. **134**, 164305 (2011). doi:10.1063/1.3582914

36. **M. Barbatti**, **Nonadiabatic dynamics with trajectory surface hopping,** WIREs: Comp. Mol. Sci. **1**, 620 (2011). doi:10.1002/wcms.64

37. **M. Barbatti**, **The role of tautomers in the UV absorption of urocanic acid**; Phys. Chem. Chem. Phys. **13**, 4686 (2011). doi:10.1039/C0CP02142C

38. **M. Barbatti**, A. J. A. Aquino, J. J. Szymczak, D. Nachtigallova, and H. Lischka, **Photodynamical Simulations of Cytosine: Characterization of the Ultra Fast Bi-Exponential UV Deactivation**; Phys. Chem. Chem. Phys.**13**, 6145 (2011). doi:10.1039/C0CP01327G

39. **M. Barbatti**, J. J. Szymczak, A. J. A. Aquino, D. Nachtigallova, and H. Lischka, **The decay mechanism of photo-excited guanine - a nonadiabatic dynamics study**; J. Chem. Phys. **134**, 014304 (2011). doi:10.1063/1.3521498

40. J. J. Szymczak, **M. Barbatti**, and H. Lischka, **Influence of the active space on CASSCF nonadiabatic dynamics simulations**; Int. J. Quantum. Chem. **111**, 3307 (2011). 10.1002/qua.22978

41. P. G. Szalay, A. J. A. Aquino, **M. Barbatti**, and H. Lischka, **Theoretical study of the excitation spectrum of azomethane**; Chem. Phys. **380**, 9 (2011). doi:10.1016/j.chemphys.2010.08.013

42. M. Ruckenbauer, **M. Barbatti**, B. Sellner, T. Muller, and H. Lischka, **Azomethane: nonadiabatic photodynamical simulations in solution**; J. Phys. Chem. A **114**, 12585 (2010). doi:10.1021/jp108844g

43. **M. Barbatti**, A. J. A. Aquino, J. J. Szymczak, D. Nachtigallova, P. Hobza, and H. Lischka, **On the relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases**; PNAS **107**, 21453 (2010). doi:10.1073/pnas.1014982107

44. D. Nachtigallova, **M. Barbatti**, J. J Szymczak, P. Hobza, and H. Lischka, **The Photodynamics of 2,4-Diaminopyrimidine in Comparison with 4-Aminopyrimidine: The Effect of Aminosubstitution**; Chem. Phys. Letters **497**, 129 (2010). doi:10.1016/j.cplett.2010.07.098

45. **M. Barbatti**, J. Pittner, M. Pederzoli, U. Werner, R. Mitric, V. Bonacic-Koutecky, H. Lischka, **Nonadiabatic dynamics of pyrrole: dependence of deactivation mechanisms on the excitation energy**; Chem. Phys. **375**, 26 (2010). doi:10.1016/j.chemphys.2010.07.014

46. M. Eckert-Maksic, M. Vazdar, M. Ruckenbauer, **M. Barbatti**, T. Müller and H. Lischka, **Matrix-Controlled Photofragmentation of Formamide: Dynamics Simulation in Argon by Nonadiabatic QM/MM Method**; Phys. Chem. Chem. Phys. **12**, 12719 (2010). doi:10.1039/C0CP00174K

47. D. Nachtigallova, T. Zeleny, M. Ruckenbauer, T. Muller, **M. Barbatti**, P. Hobza, and H. Lischka, **Does stacking restrain the photodynamics of individual nucleobases?**; J. Am. Chem. Soc.**132**, 8261 (2010). doi:10.1021/ja1029705

48. M. Ruckenbauer, **M. Barbatti**, T. Muller, and H. Lischka, **Nonadiabatic Excited-State Dynamics with Hybrid ab Initio Quantum-Mechanical/Molecular-Mechanical Methods: Solvation of the Pentadieniminium Cation in Apolar Media**; J. Phys. Chem. A **114**, 6757 (2010). doi:10.1021/jp103101t

49. B. Sellner, M. Ruckenbauer, I. Stambolić, **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **The Photodynamics of Azomethane – A Nonadiabatic Surface-Hopping Study**; J. Phys. Chem. A **114**, 8778 (2010). doi:10.1021/jp101745t

50. D. Nachtigallova, H. Lischka, J. J. Szymczak, **M. Barbatti**, P. Hobza, Z. Gengeliczki, G. Pino, M. P. Callahan, and M. S. d. Vries, **The effect of C5 substitution on the photochemistry of uracil**; Phys. Chem. Chem. Phys. **12**, 4924 (2010). doi:10.1039/b925803p

51. V. Lukes, R. Solc, **M. Barbatti**, H. Lischka, and H. F. Kauffmann, **Torsional Potentials and Full-dimensional Simulation of Electronic Absorption Spectra of para-Phenylenevinylene Oligomers Using Semiempirical Hamiltonians**; J. Theor. Comput. Chem. **9**, 249 (2010). doi:10.1142/S0219633610005645

52. Z. Gengeliczki, M. P. Callahan, N. Svadlenak, C. I. Pongor, B. Sztaray, W. L. Meerts, D. Nachtigallová, P. Hobza, **M. Barbatti**, H. Lischka, and M. S. d. Vries, **Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine**; Phys. Chem. Chem. Phys. **12**, 5375 (2010). doi:10.1039/b917852j

53. **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **The UV absorption of nucleobases: semi-classical ab initio spectra simulations**; Phys. Chem. Chem. Phys. **12**, 4959 (2010). doi:10.1039/B924956G

54. M. Vazdar, M. Eckert-Maksic, **M. Barbatti**, and H. Lischka, **Excited-state non-adiabatic dynamics simulations of pyrrole**; Mol. Phys. **107**, 845 (2009). doi:10.1080/00268970802665639

55. J. J. Szymczak, **M. Barbatti**, J. T. Soo Hoo, J. A. Adkins, T. L. Windus, D. Nachtigallova, and H. Lischka, **Photodynamics Simulations of Thymine: Relaxation into the First Excited Singlet State**; J. Phys. Chem. A **113**, 12686 (2009). doi:10.1021/jp905085x

56. J. J. Szymczak, **M. Barbatti**, and H. Lischka, **Is the Photoinduced Isomerization in Retinal Protonated Schiff Bases a Single- or Double-Torsional Process?**; J. Phys. Chem. A **113**, 11907 (2009). doi:10.1021/jp903329j

57. B. Sellner, **M. Barbatti**, and H. Lischka, **Dynamics starting at a conical intersection: Application to the photochemistry of pyrrole**; J. Chem. Phys. **131**, 024312 (2009). doi:10.1063/1.3175799

58. F. Plasser, **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **Excited-State Diproton Transfer in [2,2 '-Bipyridyl]-3,3 '-diol: the Mechanism Is Sequential, Not Concerted**; J. Phys. Chem. A **113**, 8490 (2009). doi:10.1021/Jp9032172

59. J. Pittner, H. Lischka, and **M. Barbatti**, **Optimization of mixed quantum-classical dynamics: Time-derivative coupling terms and selected couplings**; Chem. Phys. **356**, 147 (2009). doi:10.1016/j.chemphys.2008.10.013

60. I. Borges Jr, A. J. A. Aquino, **M. Barbatti**, and H. Lischka, **The electronically excited states of RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine): Vertical excitations**; Int. J. Quantum Chem. **109**, 2348 (2009). doi:10.1002/qua.22043

61. **M. Barbatti**, H. Lischka, S. Salzmann, and C. M. Marian, **UV excitation and radiationless deactivation of imidazole**; J. Chem. Phys. **130**, 034305 (2009). doi:10.1063/1.3056197

62. **M. Barbatti**, A. J. A. Aquino, H. Lischka, C. Schriever, S. Lochbrunner, and E. Riedle, **Ultrafast internal conversion pathway and mechanism in 2-(2'-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems**; Phys. Chem. Chem. Phys. **11**, 1406 (2009). doi:10.1039/b814255f

63. A. J. A. Aquino, F. Plasser, **M. Barbatti**, and H. Lischka, **Ultrafast Excited-state Proton Transfer Processes: Energy Surfaces and On-the-fly Dynamics Simulations**; Croat. Chem. Acta **82**, 105 (2009).

64. G. Zechmann and **M. Barbatti**, **Ab initio study of the photochemistry of aminopyrimidine**; Int. J. Quantum Chem. **108**, 1266 (2008).
doi: 10.1002/qua.21612

65. G. Zechmann and **M. Barbatti**, **Photophysics and Deactivation Pathways of Thymine**; J. Phys. Chem. A **112**, 8273 (2008).
doi:10.1021/jp804309x

66. J. J. Szymczak, **M. Barbatti**, and H. Lischka, **Mechanism of Ultrafast Photodecay in Restricted Motions in Protonated Schiff Bases: The Pentadieniminium Cation**; JCTC **4**, 1189 (2008).
doi:10.1021/ct800148n

67. C. Schriever, **M. Barbatti**, K. Stock, A. J. A. Aquino, D. Tunega, S. Lochbrunner, E. Riedle, R. de Vivie-Riedle, and H. Lischka, **The interplay of skeletal deformations and ultrafast excited-state intramolecular proton transfer: Experimental and theoretical investigation of 10-hydroxybenzo[h]quinoline**; Chem. Phys. **347**, 446 (2008).
doi:10.1016/j.chemphys.2007.10.021

68. V. Lukes, R. Solc, **M. Barbatti**, M. Elstner, H. Lischka, and H.-F. Kauffmann, **Torsional potentials and full-dimensional simulation of electronic absorption and fluorescence spectra of para-phenylene oligomers using the semiempirical self-consistent charge density-functional tight binding approach**; J. Chem. Phys. **129**, 164905 (2008).
doi:10.1063/1.2998523

69. **M. Barbatti**, M. Ruckenbauer, J. J. Szymczak, A. J. A. Aquino, and H. Lischka, **Nonadiabatic excited-state dynamics of polar p-systems and related model compounds of biological relevance**; Phys. Chem. Chem. Phys. **10**, 482 (2008).
doi:10.1039/b709315m

70. **M. Barbatti** and H. Lischka, **Nonadiabatic Deactivation of 9H-Adenine: A Comprehensive Picture Based on Mixed Quantum-Classical Dynamics**; J. Am. Chem. Soc. **130**, 6831 (2008).
doi:10.1021/ja800589p

71. **M. Barbatti**, S. Belz, M. Leibscher, H. Lischka, and J. Manz, **Sensitivity of femtosecond quantum dynamics and control with respect to non-adiabatic couplings: Model simulations for the cis-trans isomerization of the dideuterated methaniminium cation**; Chem. Phys. **350**, 145 (2008).
doi:10.1016/j.chemphys.2008.01.053

72. **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **Theoretical investigation of the mode-specific induced non-radiative decay in 2-pyridone**; Chem. Phys. **349**, 278 (2008).
doi:10.1016/j.chemphys.2008.02.007

73. I. Antol, M. Vazdar, **M. Barbatti**, and M. Eckert-Maksic, **The effect of protonation on the photodissociation processes in formamide - An ab initio surface hopping dynamics study**; Chem. Phys. **349**, 308 (2008).
doi:10.1016/j.chemphys.2008.01.026

74. I. Antol, **M. Barbatti**, M. Eckert-Maksić, and H. Lischka, **Quantum chemical calculations of electronically excited states: formamide, its protonated form and alkali cation complexes as case studies**; Monatshefte für Chemie / Chemical Monthly **139**, 319 (2008).
doi:10.1007/s00706-007-0803-2

75. C. C. Turci, A. B. Rocha, **M. Barbatti**, C. E. Bielschowsky, I. G. Eustatiu, T. Tyliszczak, G. Cooper, and A. P. Hitchcock, **Experimental and theoretical study of S 2p and C 1s generalized oscillator strengths in CS_2**; J. Electron Spectrosc. Relat. Phenom. **155**, 21 (2007).
doi:10.1016/j.elspec.2006.12.001

76. M. Schreiber, **M. Barbatti**, S. Zilberg, H. Lischka, and L. Gonzalez, **An ab initio study of the excited states, isomerization energy profiles and conical intersections of a chiral cyclohexylidene derivative**; J. Phys.

Chem. A **111**, 238 (2007).
doi:10.1021/jp066090x

77. I. G. Eustatiu, T. Tyliszczak, G. Cooper, A. P. Hitchcock, C. C. Turci, A. B. Rocha, **M. Barbatti**, and C. E. Bielschowsky, **Experimental and theoretical study of S 2p and C 1s spectroscopy in CS_2**; J. Electron Spectrosc. Relat. Phenom. **156-158**, 158 (2007).
doi:10.1016/j.elspec.2006.12.065

78. **M. Barbatti** and H. Lischka, **Can the Nonadiabatic Photodynamics of Aminopyrimidine Be a Model for the Ultrafast Deactivation of Adenine?**; J. Phys. Chem. A **111**, 2852 (2007).
doi:10.1021/jp070089w

79. **M. Barbatti**, G. Granucci, M. Persico, M. Ruckenbauer, M. Vazdar, M. Eckert-Maksic, and H. Lischka, **The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems**; J. Photochem. Photobiol., A **190**, 228 (2007).
doi:10.1016/j.jphotochem.2006.12.008

80. I. Antol, M. Eckert-Maksic, **M. Barbatti**, and H. Lischka, **Simulation of the photodeactivation of formamide in the n_O-π* and π-π* states: An ab initio on-the-fly surface-hopping dynamics study**; J. Chem. Phys. **127**, 234303 (2007).
doi:10.1063/1.2804862

81. G. Zechmann, **M. Barbatti**, H. Lischka, J. Pittner, and V. Bonačić-Koutecký, **Multiple pathways in the photodynamics of a polar π-bond: A case study of silaethylene**; Chem. Phys. Lett. **418**, 377 (2006).
doi:10.1016/j.cplett.2005.11.015

82. M. Eckert-Maksic, M. Vazdar, **M. Barbatti**, H. Lischka, and Z. B. Maksic, **Automerization reaction of cyclobutadiene and its barrier height: An ab initio benchmark multireference average-quadratic coupled cluster study**; J. Chem. Phys. **125**, 064310 (2006).
doi:10.1063/1.2222366

83. **M. Barbatti**, M. Vazdar, A. J. A. Aquino, M. Eckert-Maksic, and H. Lischka, **The nonadiabatic deactivation paths of pyrrole**; J. Chem. Phys. **125**, 164323 (2006).
doi:10.1063/1.2363376

84. **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **Ultrafast two-step process in the non-adiabatic relaxation of the $CH_2NH_2^+$ molecule**; Mol. Phys. **104**, 1053 (2006).
doi:10.1080/00268970500417945

85. A. J. A. Aquino, **M. Barbatti**, and H. Lischka, **Excited-state properties and environmental effects for protonated Schiff bases: A theoretical study**; Chemphyschem **7**, 2089 (2006).
doi:10.1002/cphc.200600199

86. **M. Barbatti**, M. Ruckenbauer, and H. Lischka, **The photodynamics of ethylene: A surface-hopping study on structural aspects**; J. Chem. Phys. **122**, 174307 (2005).
doi:10.1063/1.1888573

87. **M. Barbatti**, A. B. Rocha, and C. E. Bielschowsky, **Young-type interference pattern in molecular inner-shell excitations by electron impact**; Phys. Rev. A **72** (2005).
doi:10.1103/PhysRevA.72.032711

88. **M. Barbatti**, G. Granucci, M. Persico, and H. Lischka, **Semiempirical molecular dynamics investigation of the excited state lifetime of ethylene**; Chem. Phys. Lett. **401**, 276 (2005).
doi:10.1016/j.cplett.2004.11.069

89. **M. Barbatti**, A. J. A. Aquino, and H. Lischka, **A multireference configuration interaction investigation of the excited-state energy surfaces of fluoroethylene (C_2H_3F)**; J. Phys. Chem. A **109**, 5168 (2005).
doi:10.1021/jp050834+

90. **M. Barbatti**, A. B. Rocha, and C. E. Bielschowsky, **Generalized oscillator strength for core excitations of nitrous oxide**; Chem. Phys. **299**, 83 (2004).
doi:10.1016/j.chemphys.2003.11.043

91. **M. Barbatti**, J. Paier, and H. Lischka, **Photochemistry of ethylene: A multireference configuration interaction investigation of the excited-state energy surfaces**; J. Chem. Phys. **121**, 11614 (2004). doi:10.1063/1.1807378

92. **M. Barbatti** and M. A. C. Nascimento, **Vibrational analysis of small H_n^+ hydrogen clusters**; J. Chem. Phys. **119**, 5444 (2003). doi:10.1063/1.1599350

93. **M. Barbatti** and M. A. C. Nascimento, **On the formation mechanisms of hydrogen ionic clusters**; Braz. J. Phys. **33**, 792 (2003). doi:10.1590/S0103-97332003000400032

94. A. P. Hitchcock, S. Johnston, T. Tyliszczak, C. C. Turci, **M. Barbatti**, A. B. Rocha, and C. E. Bielschowsky, **Generalized oscillator strengths for C 1s excitation of acetylene and ethylene**; J. Electron Spectrosc. Relat. Phenom. **123**, 303 (2002). doi:10.1016/S0368-2048(02)00029-4

95. **M. Barbatti**, G. Jalbert, and M. A. C. Nascimento, **Clustering of hydrogen molecules around a molecular cation: The $Li_3^+(H_2)_n$ clusters (n=1-6)**; J. Phys. Chem. A **106**, 551 (2002). doi:10.1021/jp013159m

96. F. Gobet, B. Farizon, M. Farizon, M. J. Gaillard, S. Louc, N. Goncalves, **M. Barbatti**, H. Luna, G. Jalbert, N. V. C. Faria, M. C. Bacchus-Montabonel, J. P. Buchet, M. Carre, and T. D. Mark, **Event-by-event analysis of collision-induced cluster-ion fragmentation: Sequential monomer evaporation versus fission reactions**; Phys. Rev. Lett. **86**, 4263 (2001). doi:10.1103/PhysRevLett.86.4263

97. **M. Barbatti**, G. Jalbert, and M. A. C. Nascimento, **The effects of the presence of an alkaline atomic cation in a molecular hydrogen environment**; J. Chem. Phys. **114**, 2213 (2001). doi:10.1063/1.1338978

98. **M. Barbatti**, G. Jalbert, and M. A. C. Nascimento, **The structure and the thermochemical properties of the $H_3^+(H_2)_n$ clusters (n=8-12)**; J. Chem. Phys. **114**, 7066 (2001). doi:10.1063/1.1360198

99. **M. Barbatti**, G. Jalbert, and M. A. C. Nascimento, **Isomeric structures and energies of H_n^+ clusters (n=13, 15, and 17)**; J. Chem. Phys. **113**, 4230 (2000). doi:10.1063/1.1288381

100. **M. Barbatti**, N. V. C. Faria, J. C. Acquadro, and R. Donangelo, **Dependence on the incident angle of the electronic energy loss of planarly channeled fast ions**; Nucl. Instrum. Methods Phys. Res., Sect. B **149**, 425 (1999). doi:10.1016/S0168-583X(98)00935-5

101. **M. Barbatti**, L. P. G. de Assis, G. Jalbert, L. F. S. Coelho, I. Borges, and N. V. C. Faria, **Collisional fragmentation of fast HeH^+ ions: The $He_2^+ + H^-$ channel**; Phys. Rev. A **59**, 1988 (1999). doi:10.1103/PhysRevA.59.1988

Book Chapters and Full Papers in Proceedings

1. **M. Barbatti**, R. Crespo-Otero, **Surface Hopping Dynamics with DFT Excited States**, in *Density-functional methods for excited states*, edited by N. Ferré, M. Filatov, M. Huix-Rotllant, Top. Curr. Chem. in press (Springer, 2015). doi:10.1007/128_2014_605

2. **M. Barbatti**, A. C. Borin, S. Ullrich, **Photoinduced processes in nucleic acids**, in *Photoinduced processes in nucleic acids*, Vol. 1, edited by M. Barbatti, A. C. Borin, S. Ullrich, Top. Curr. Chem. **355**, 1 (2015). doi:10.1007/128_2014_569

3. M. Pederzolli, **M. Barbatti**, H. Lischka, J. Pittner, **Cis-trans photoisomerization of azobenzene excited to the S_1 state: An ab initio QM/MM molecular dynamics study**, in *Proceedings of SPIE*, Vol. 8463,

Nanoengineering: Fabrication, Properties, Optics, and Devices IX, 846318 (2012).
doi: 10.1117/12.930478

4. **M. Barbatti**, M. Ruckenbauer, J. J. Szymczak, B. Sellner, M. Vazdar, I. Antol, M. Eckert-Maksic, H. Lischka, **Model systems for dynamics of π-conjugated molecules in excited states**, in *Handbook of Computational Chemistry*, edited by J. Leszczynski (Springer, Netherlands, 2012), p. 1175
doi:10.1007/978-94-007-0711-5_33

5. **M. Barbatti**, R. Shepard, H. Lischka, **Computational and methodological elements for nonadiabatic trajectory dynamics simulations of molecules**, in *Conical Intersections: Theory, Computation and Experiment*, edited by W. Domcke, D. R. Yarkony, and H. Koppel (World Scientific, Singapore, 2011), p. 415.
doi:10.1142/9789814313452_0011

6. M. Eckert-Maksic, I. Antol, M. Vazdar, **M. Barbatti**, H. Lischka, **Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond**, in *Kinetics and Dynamics:* Challenges and Advances in Coutational Chemistry and Physics, edited by P. Paneth and A. Dybala-Defratyka (Springer, Netherlands, 2010), p. 77.
doi:10.1007/978-90-481-3034-4_3

7. **M. Barbatti**, B. Sellner, A. J. A. Aquino, H. Lischka, **Nonadiabatic excited-state dynamics of aromatic heterocycles: toward the time-resolved simulation of nucleobases**, in *Radiation Induced Molecular Phenomena in Nucleic Acid*, edited by M. K. Shukla and J. Leszczynski (Springer, Netherlands, 2008), p. 209.
doi:10.1007/978-1-4020-8184-2_8

8. M. Ruckenbauer, I. Brandic, S. Benkner, W. Gansterer, O. Gervasi, **M. Barbatti**, H. Lischka, **Nonadiabatic ab initio surface-hopping dynamics calculation in a grid environment - First experiences**, in *Lecture Notes in Computer Science*, edited by O. Gervasi and M. Gavrilova (Springer-Verlag, Berlin, 2007), Vol. 4705 LNCS, p. 281.
doi:10.1007/978-3-540-74472-6_22

9. H. Lischka, A. J. A. Aquino, **M. Barbatti**, M. Solimannejad, **High-level quantum chemical methods for the study of photochemical processes**, in *Computational Science and Its Applications - Iccsa 2005, Pt 1* (2005), Vol. 3480, p. 1004.
doi:10.1007/11424758_104

Manuals, White Papers, and Other Publications

1. M. Ruckenbauer, D. Fazzi, and **M. Barbatti**, **A tutorial for Newton-X** (2008-2013).
www.univie.ac.at/newtonx/docs/tutorial.pdf

2. **M. Barbatti**, **Newton-X documentation** (2008-2013).
www.univie.ac.at/newtonx/nx-docs-1_4.pdf

3. B. Sellner, J. J. Szymczak, F. Plasser, **M. Barbatti**, A tutorial for Columbus (2008).
www.univie.ac.at/columbus/documentation/tutorial.pdf

4. **M. Barbatti**, **A Filosofia Natural à Época de Newton (Natural philosophy at the Newton's age)**, Revista Brasileira de Ensino de Física, 21, 153 (1999).

5. **M. Barbatti**, **Conceitos Físicos e Metafísicos no Jovem Newton: Uma Leitura do de Gravitatione (Physical and metaphysical concepts for the young Newton)**, Revista da Sociedade Brasileira de História da Ciência, 17, 59 (1997).

Editorial Works

1. M. Barbatti, A. C. Borin, S. Ullrich (Eds.), **Photoinduced processes in nucleic acids Vol. II: DNA Fragments and Phenomenological Aspects** (Springer, 2015).
ISBN 978-3-319-13272-3

2. M. Barbatti, A. C. Borin, S. Ullrich (Eds.), **Photoinduced processes in nucleic acids Vol. I: Nucleobases in the Gas Phase and Solvated** (Springer, 2015).
ISBN 978-3-319-13371-3.

3. **M. Barbatti**, H. Köppel, R. Shepard, P. G. Szalay (Guest eds.), **Electron correlation and molecular dynamics for excited states and photochemistry**, Chem. Phys. **349** (2008).
doi:10.1016/j.chemphys.2008.05.017

Web Contents

1. Light and Molecules – www.barbatti.org: website and blog with general information and the latest news on my group's research.
2. Much Bigger Outside – mariobarbatti.wordpress.com: personal blog on general scientific topics.

Theses

1. **M. Barbatti**, **Ultrafast Molecular Dynamics in Excited States Using Mixed Quantum-Classical Approaches**, Habilitation Thesis (University of Vienna, Vienna, 2008).

2. **M. Barbatti**, **Formação de agregados de hidrogênio em torno de cátions atômicos e moleculares (Hydrogen clustering around atomic and molecular cations)**, Ph.D. Thesis, advisor: G. Jalbert (Federal University of Rio de Janeiro, Rio de Janeiro, 2001).

3. **M. Barbatti**, **Perda de Energia de Ions Rápidos de Hélio em Germânio e Silício sob Regime de Canalização (Energy loss of fast He ions channeled through Ge and Si crystals)**, Master Thesis, advisor: N. V. de Castro Faria (Federal University of Rio de Janeiro, Rio de Janeiro, 1997).