**Surname** BICZYSKO
**Name** MALGORZATA AGNIESZKA
**Gender** F
**Born** WROCLAW, POLAND, 22 March 1970
**E-mail:** biczysko@shu.edu.cn
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**Scopus Author ID:** 55892951700

# *Curriculum Vitae*

**Academic Degrees:**

## 11/ 2013

Italian National Scientific Qualification as Associate Professor in Chemistry (03/A2: Models and Methodologies for Chemical sciences).

## 29 / 06 / 2000

PhD in Theoretical Chemistry, University of Wrocław, Poland, Faculty of Chemistry, PhD Supervisor: Prof. Zdzislaw Latajka, Thesis: "Theoretical investigations of environmental effect on proton position in hydrogen bridge in hydrogen bonded complexes XH-$NH_3$ (X=F, Cl, Br)".

## 28 / 07 / 1994

M.Sc in Chemistry, vote 5/5, Faculty of Mathematic, Physics and Chemistry, University of Wrocław, Poland. Supervisor: Dr. K. Romanowska, Thesis: "QSAR-graph-theoretical study of ionic transport in biological systems".

**PROFESSIONAL EXPERIENCE:**

2015- present Asscociate Professor at International Centre for Quantum and Molecular Structures, College of Sciences, Shanghai University.

2014-2015 Researcher at the Institute of Chemistry of OrganoMetallic Compounds of the National Research Council of Italy (CNR-ICCOM)

2013-2014 Post-doctoral position (Assegno per la collaborazione ad attivita di ricerca) Scuola Normale Superiore, Pisa. Research project "Development, validation and application of computational approaches for simulation of accurate, high- and medium-resolution vibrational and vibronic spectra", supervisor Prof. Vincenzo Barone.

2011-2013 Senior Post-doctoral position (Collaboratore a progetto) Center for Nanotechnology Innovation @NEST Istituto Italiano di Tecnologia, Research project "Photoactivatable linkers for controlled NIR uncaging".

2009-2011 Post-doctoral position (Assegno per la collaborazione ad attivita di ricerca), Università degli Studi di Napoli "Federico II", Research project "Sviluppo ed applicazione di nuove strategie computazionali multi-scala per lo studio dei processi fotochimici in biomolecole verso la progettazione in silico di bionanosistemi.", supervisors: Prof. Vincenzo Barone e Prof. Orlando Crescenzi.

2006 - 2008 Post-doctoral position (Assegno per la collaborazione ad attivita di ricerca), l'Università degli Studi di Napoli "Federico II", within the Project PON S.Co.P.E, Research project "Sviluppo ed Implementazione di Protocolli Computazionali per la Simulazione di Sistemi e Processi nel Campo delle Scienze della Vita", supervisor: Prof. Vincenzo Barone, Project coordinator: Prof. G. Marucci.

2004-2006 Post-doctoral position, University of Coimbra (Portugal), European program Marie Curie Research Training Networks 'Predicting Catalysis: Understanding Ammonia Synthesis from First-Principles Calculations" (Contract No HPRN-CT-2002-00170). Supervisor: Prof. António J. C. Varandas, Project coordinator Prof. G. J. Kroes, Leiden University, Leiden, Netherlands.

2003-2004 Post-doctoral position, University of Helsinki (Finland), European program TMR Research Training Networks 'THEONET II' (Contract No. HPRN-CT-1999-00005) "Theoretical studies of Electronic and Dynamical Properties in Molecules and Clusters: Computational Study of the Adsorption of Ammonia on the Ni(111) Surface", supervisor Prof. Lauri Halonen, Project coordinator Prof. Pavel Rosmus, Universite Marne la Vallee, Paris, France.

2000-2003 Post-doctoral position, Università di Bologna, European program TMR Research Training Networks 'THEONET II' (Contract No. HPRN-CT-1999-00005) "Theoretical studies of Electronic and Dynamical Properties in Molecules and Clusters: Rovibronic levels for systems showing the Renner-Teller effect and large spin-orbit coupling", supervisor Prof. Paolo Palmieri, Project coordinator Prof. Pavel Rosmus, Universite Marne la Vallee, Paris, France.

**REFEREE, EDITORIAL & Scientific Committees**

**Editor of Journal of Molecular Structure (Elsevier, IF: 2.12) since July 2016**

**Editorial Board member of International Journal of Quantum Chemistry (Wiley, IF: 2.92) since March 2018**

**Review Committee Jury member for The Final of the Belt and Road International Special Event Contest of the 15th Challenge Cup National College Students' Extracurricular Academic Science and Technology Works Contest, Shanghai (16, November, 2018)**

**Member of international Ph.D. Board (2019-2020) for Astrochemistry (2018-2019 for Methods and Models for Molecular Sciences) at Scuola Normale Supertiore (Pisa, Italy)**

Referee for journals: Journal of American Chemical Society, Accounts of Chemical Research, Chemical Reviews, Chemical Science, RSC Advances, Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Journal of Chemical Physics, Chemical Physics, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy. ChemPhysChem, J. Molecular Spectroscopy, Chemical Physics Letters, Journal of Chemical Theory and Computations, Theoretical Chemistry Accounts, Computational and Theoretical Chemistry, Journal of Luminescence

Evaluation of Research Projects for: "Progetti di Ricerca di Interesse Nazionale" (PRIN) funded by the Italian Ministry of University and Research (MIUR), the University of Turin, Italy; Scuola Normale Superiore, Pisa, Italy.

**RESEARCH ACTIVITIES**

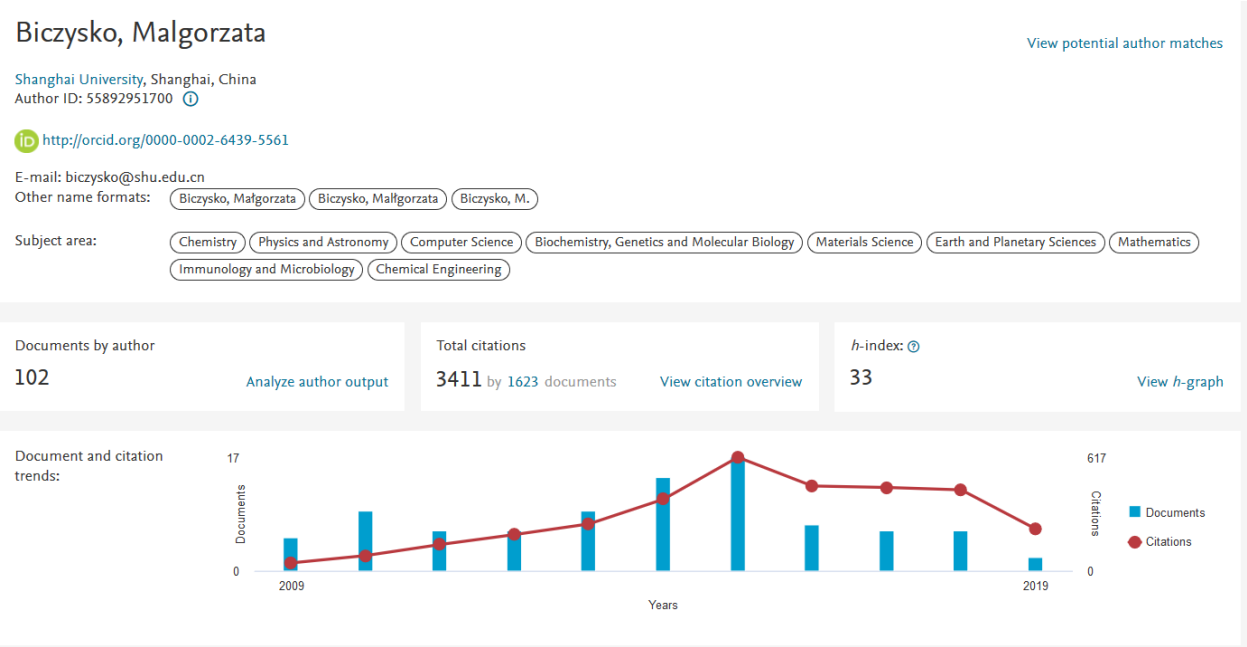
MB research activity is focused on computational spectroscopy and aim at the definition of tailored computational protocols allowing simulations and detailed analysis of spectroscopic phenomena for non-periodic molecular systems of increasing complexity, featuring dispersion interactions, hydrogen bonding, variable local stereochemistry-conformation, and chirality. Her expertise is mainly related to the development, validation and applications of computational spectroscopy approaches to simulations of vibrational anharmonic and vibrationally resolved electronic spectra line-shapes. Unprecedented accuracy of such studies, allowing a deeper understanding of experimental results and the underlying phenomena, has been already witnessed for large range of molecular systems and spectroscopies.

MB has effectively coordinated several collaborative projects, involving other experimental and theoretical research groups. She also established a large collaborative network with theoretical and

experimental spectroscopic research groups, mainly from Europe, US and China. She actively participated to several international projects, mainly founded by European Union, including also preparation of grant proposals, project management and reporting. For the CM1002 COST Action-CoDECS (COnvergent Distributed Environment for Computational Spectroscopy), she has been responsible for the scientific and administrative organization, budget planning and reporting on behalf of Management Committee. This project has been included as a ‘flag-ship’ success story in the COST Annual Report 2014.

## PUBLICATION LIST

*Journal Impact Factor (IF), Citations ISI Web of Science (ISI), Scopus (S) and Google Scholar (GS)*
**Citations report as of 22/06/2019**




**2019**

1. H. Zhang, J. Krupa, M. Wierzejewska, **M. Biczysko**, "The Role of Dispersion and Anharmonic Corrections in Conformational Analysis of Flexible Molecules: the Allyl Group Rotamerization of Matrix Isolated Safrole" Phys. Chem. Chem. Phys. DOI: 10.1039/C9CP00926D, 2019 (IF: 3.906, ISI: 0, S: 0, GS:0, **corresponding author**)
2. A. Bil, J. Gregoliński, **M. Biczysko** "Internal Hydrogen Bond Influences the Formation of [2+2] Schiff Base Macrocycle: Open-Chain Vs. Hemiaminal and Macrocycle Forms" Eur. J. Org. Chem. 2019, 2243 – 2252, 2019 (IF: 2.882, ISI: o, S: 0, GS: 0)

**2018**

3. M. Biczysko, J. Krupa, M. Wierzejewska, "Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light" Faraday Discussions, 212, 421-441, 2018 (IF: 3.427 ISI: 0, S: 0, GS:0, **corresponding author**)
4. Z. Bacic, D. Benoit, **M. Biczysko**,et al. Molecules in confinement in clusters, quantum solvents and matrices: general discussion, Faraday discussions, 212, 569-601, 2018 (IF: 3.427 ISI: 0, S: 0, GS)

5. C. Degli Esposti, L. Dore, C. Puzzarini, **M. Biczysko**, J. Bloino, L. Bizzocchi, V. Lattanzi, J.-U. Grabow "Accurate rest frequencies for propargylamine in the ground and low-lying vibrational states" A&A 615, A176, 2018 (IF: 5.014, ISI: 0, S: 0, GS:0)
6. A. Bil, Z. Latajka, **M. Biczysko** "Hydrogen detachment driven by a repulsive $^1\pi\sigma^*$ state-an electron localization function study of 3-amino-1,2,4-triazole" Phys. Chem. Chem. Phys. 20, 5210-5216, 2018 (IF: 4.123, ISI: 0, S: 0, GS:0, **corresponding author**)
7. Z. Jiang, **M. Biczysko**, N. W. Moriarty "Accurate geometries for "mountain pass" regions of the Ramachandran plot using quantum chemical calculations" Proteins: Structure, Function, and Bioinformatics, 86, 273-278, 2018 (IF: 2.289, ISI:0, S:0, GS:0)
8. **M. Biczysko**, J. Bloino, C. Puzzarini "Computational challenges for astrochemistry" WIREs Comput Mol Sci 8, e1349, 2018 (IF: 14.016, ISI: 2, S:2, GS:5)

**2017**

9. M. H. Palmer, **M. Biczysko**, K. A. Peterson, C. S. Stapleton, S. P. Wells "Structural and Vibrational Properties of Iodopentafluorobenzene: A Combined Raman and Infrared Spectral and Theoretical Study" Journal of Physical Chemistry A 121, pp 7917 – 7924, 2017 (IF: 2.847, ISI:0, S:0, GS:0, **corresponding author**)
10. M. H. Palmer, M. Biczysko, A. Baiardi, M. Coreno, M. De Simone, C. Grazioli, S. V. Hoffmann, N. C. Jones, K. A. Peterson 'The ionic states of difluoromethane: A reappraisal of the low energy photoelectron spectrum including ab initio configuration interaction computations" Journal of Chemical Physics 147 , 074305, 2017 (IF: 2.965, ISI:0 ; S:2; GS:2, **corresponding author**)
11. C. Puzzarini , **M. Biczysko** , K. A. Peterson , J. S. Francisco , R. Linguerri "Accurate spectroscopic characterization of the HOC(O)O radical: a route toward its experimental identification" Journal of Chemical Physics 147, 024302, 2017 (IF: 2.965, ISI:0 ; S:3; GS:3)
12. A. Pietropolli Charmet, P. Stoppa, S. Giorgianni, J. Bloino, N. Tasinato, I. Carnimeo, **M. Biczysko**, and C. Puzzarini "Accurate Vibrational−Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study" Journal of Physical Chemistry A 121, 3305 – 3317, 2017 (IF: 2.847, ISI:6, S:6, GS:6)
13. M. H. Palmer, S. Vrønning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, K. A. Peterson, A. Baiardi, T. Zhang, and **M. Biczysko** "A combined theoretical and experimental study of the valence and Rydberg states of iodopentafluorobenzene", Jounal of Chemical Physics,

146, 174301, 2017 (IF: 2.965, ISI:0 ; S:2; GS:2, **corresponding author**)

14. M. H Palmer, M. Coreno, M. De Simone, S. Vrønning Hoffmann, N. C Jones, C. Grazioli, K. A Peterson, A. Baiardi, T. Zhang, **M. Biczysko** "A combined theoretical and experimental study of the ionic states of iodopentafluorobenzene" Jounal of Chemical Physics 146, 084302, 2017 (IF: 2.965, ISI:1 ; S:2; GS:1, **corresponding author**)

**2016**

15. J Bloino, A Baiardi, **M Biczysko** "Aiming at an accurate prediction of vibrational and electronic spectra for medium-to-large molecules: An overview" International Journal of Quantum Chemistry, 116, 1543 – 1574, 2016, (IF: 2.184, ISI: 41; S: 48; GS: 56, **corresponding author**)
16. J. R. Reimers, **M. Biczysko**, D. Bruce, D.F. Coker, T.J. Frankcombe et al., "Challenges facing an understanding of the nature of low-energy excited states in photosynthesis" Biochimica et Biophysica Acta (BBA)-Bioenergetics 1857, 1627-1640, 2016 (IF: ISI: 32; S: 30; GS: 34)
17. M. Hodecker, **M. Biczysko**, A. Dreuw, V. Barone "Simulation of Vacuum UV Absorption and Electronic Circular Dichroism Spectra of Methyl Oxirane: The Role of Vibrational Effects" Journal of Chemical Theory and Computation 12, 2820, 2016 (IF:5.301, ISI: 16; S: 20; GS:25, **corresponding author**)
18. M. H. Palmer, T. Ridley, S. Vrønning Hoffmann, N. C Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang, **M. Biczysko**, A. Baiardi, K. Peterson "Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene" Palmer, M.H., Ridley, T., Journal of Chemical Physics 144, 204305, 2016 (IF: 3.122 ISI:5; S:7, GS:6, **corresponding author** )
19. M. H. Palmer, T. Ridley, S. Vrønning Hoffmann, N. C Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang, **M. Biczysko**, A. Baiardi, K. Peterson "Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene" Journal of Chemical Physics 144, 124302 2016, (IF: 3.122 ISI:3; S:3, GS:1, **corresponding author**)
20. T. Fornaro, M. Biczysko, J. Bloino, V. Barone "Reliable Vibrational Wavenumbers for C=O and N-H Stretchings of Isolated and Hydrogen-bonded Nucleic Acid Bases" Phys. Chem. Chem. Phys. 18, 8479, 2016, (IF: 4.493, ISI: 5; S: 7; GS: 5, **corresponding author** )

**2015**

21. J. Bloino, M. Biczysko, V. Barone "Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism and Raman Optical Activity" J. Phys. Chem. A 119, 11862−11874, 2015 (IF: 3.122 ISI:10; S:16, GS:21, **corresponding author**)

22. V. Barone, **M. Biczysko**, C. Latouche, A. Pasti "Virtual eyes for technology and cultural heritage: towards computational strategy for new and old indigo-based dyes" Theoretical Chemistry Accounts 134 (12), 1-14, 2015 (IF: 2.233., ISI:2; S:2, GS:4, **corresponding author**)
23. H. Kvapilova, A. Vlcek, V. Barone, **M. Biczysko,** S. Zalis "Anharmonicity Effects in IR Spectra of [Re(X)(CO)3( α -diimine)] ( α -diimine= 2,2'-bipyridine or pyridylimidazo[1,5-a]pyridine; X=Cl or NCS) Complexes in Ground- and Excited Electronic States" J. Phys. Chem. A, 119 (40), pp 10137–10146 2015 (IF: 2.775, ISI:5; S:7, GS:7, **corresponding author**)
24. T. Fornaro, D. Burini, **M. Biczysko**, V. Barone "Hydrogen-Bonding Effects on Infrared Spectra from Anharmonic Computations: Uracil−Water Complexes and Uracil Dimers" J. Phys. Chem. A 119, 4224–4236, 2015 (IF: 2.775, ISI:14; S:25, GS:18, **corresponding author**)
25. EE Najbauer, G Bazsó, R Apóstolo, R Fausto, **M Biczysko**, V Barone, G. Tarczay "Identification of Serine Conformers by Matrix Isolation IR Spectroscopy Aided by Near Infrared Laser Induced Conformational Change, 2D Correlation Analysis, and Quantum Mechanical Anharmonic Computations" J. Phys. Chem. B 119, 10496–10510, 2015 (IF:3.302 ISI:4, S:7, GS:6 )
26. M. H. Palmer, T. Ridley, S. Vrønning Hoffmann, N. C Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang, **M. Biczysko**, A. Baiardi, K. Peterson "Interpretation of the photoelectron, ultraviolet, and vacuum ultraviolet photoabsorption spectra of bromobenzene by ab initio configuration interaction and DFT computations" J. Chem. Phys. 143, 164303, 2015 (IF: 3.122 ISI:4; S:8, GS:1, **corresponding author**)
27. V. Barone, F. Bellina, **M. Biczysko**, J. Bloino, T. Fornaro, C. Latouche, M. Lessi, G. Marianetti, P. Minei, A. Panattoni A. Pucci "Toward the design of alkynylimidazole fluorophores: computational and experimental characterization of spectroscopic features in solution and in poly(methyl methacrylate) Phys. Chem. Chem. Phys., 17, 26710-26723, 2015, (IF: 4.493. ISI:3, S:6, GS:7, **corresponding author**)
28. V Barone, **M Biczysko**, J Bloino, P Cimino, E Penocchio, C Puzzarini "The CC/DFT Route towards Accurate Structures and Spectroscopic Features for Observed and Elusive Conformers of Flexible Molecules: Pyruvic Acid as Case Study" J. Chem. Theory Comput. 11, 4342-4363, 2015 (IF: 5.389, ISI:019 S:25, GS:19)
29. C Puzzarini, **M Biczysko** "Microsolvation of 2-Thiouracil: Molecular Structure and Spectroscopic Parameters of the Thiouracil-Water Complex" J. Phys. Chem. A 119, 5386–5395 , 2015 (IF:2.775 ISI:0; S:9, GS:8)

30. V. Barone, **M. Biczysko**, C. Puzzarini "Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules" Acc. Chem. Res. 48, 1413–1422, 2015 (IF: 24.348, ISI:12; S:17, GS:14, **corresponding author**)
31. M. H. Palmer, T. Ridley, S. Vrønning Hoffmann, N. C Jones, M. Coreno, M.de Simone, C. Grazioli, **M. Biczysko**, A. Baiardi, P. Limão-Vieira "Interpretation of the vacuum ultraviolet photoabsorption spectrum of iodobenzene by ab initio computations" J. Chem. Phys. 142, 13430, 2015 (IF: 3.122, ISI:4; S:3, GS:8, **corresponding author**)
32. M. H. Palmer, T. Ridley, S. Vrønning Hoffmann, N. C Jones, M. Coreno, M.de Simone, C. Grazioli, **M. Biczysko**, A. Baiardi "The ionic states of iodobenzene studied by photoionization and ab initio configuration interaction and DFT computations" J. Chem. Phys. 142, 134301, 2015 (IF: 3.122 ISI:6; S:5, GS:11, **corresponding author**)
33. M. Piccardo, E. Penocchio, C. Puzzarini, **M. Biczysko**, V. Barone "Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules" J. Phys. Chem. A, 119, 2058 – 2082, 2015 (IF:2.775 ISI:25; S:32, GS:24)
34. T Fornaro, I Carnimeo, **M Biczysko** "Towards Feasible and Comprehensive Computational Protocol for Simulation of the Spectroscopic Properties of Large Molecular Systems: The Anharmonic Infrared Spectrum of Uracil in the Solid State by Reduced Dimensionality/Hybrid VPT2 Approach" J. Phys. Chem. A 119, 5313–5326, 2015 (IF:2.775 ISI:7; S:10, GS:7, **corresponding author**)
35. I Reva, C M. Nunes, **M Biczysko**, R Fausto "Conformational Switching in Pyruvic Acid Isolated in Ar and N2 Matrixes: Spectroscopic Analysis, Anharmonic Simulation, and Tunneling" J. Phys. Chem. A, 119, 2614 – 2627 , 2015 (IF:2.775 ISI:20; S:26, GS:23)
36. D Licari, A Baiardi, **M Biczysko**, F Egidi, C Latouche, V Barone "Implementation of a graphical user interface for the virtual multifrequency spectrometer: The VMS-Draw tool" J. Comp. Chem. 36, 321-334, 2015 (IF: 3.601, ISI:29, S:33, GS:33, **Cover article**)

**2014**

37. C. Puzzarini, A. Ali, **M. Biczysko**, V. Barone "Accurate Spectroscopic Characterization of Protonated Oxirane: A Potential Prebiotic Species in Titan's Atmosphere" The Astrophysical Journal 792 (2), 118, 2014 (IF: 6.733, ISI:4, S:7, GS:5)
38. V. Barone, **M. Biczysko**, M. Borkowska-Panek, J. Bloino "A Multifrequency Virtual Spectrometer

for Complex Bio-Organic Systems: Vibronic and Environmental Effects on the UV/Vis Spectrum of Chlorophyll a" ChemPhysChem, 15, 3355-3364, 2014 (IF: 3.360 ISI:8, S:11, GS:16, **corresponding author**)

39. V. Barone, **M. Biczysko**, J. Bloino, C. Puzzarini "Accurate molecular structures and infrared spectra of trans-2, 3-dideuterooxirane, methyloxirane, and trans-2, 3-dimethyloxirane" J. Chem. Phys. 141 (3), 034107, 2014 (IF: 3.122, ISI:18, S:27, GS:22, **corresponding author**)
40. C. Puzzarini, E. Penocchio, **M. Biczysko**, V. Barone "Molecular Structure and Spectroscopic Signatures of Acrolein: theory meets experiment." J. Phys. Chem. A 118, 6648–6656, 2014 (IF:2.771 ISI:12; S:13, GS:14)
41. V. Barone, **M. Biczysko**, J. Bloino, L. Carta, A. Pedone "Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: Coumarin derivatives as test cases" Comput. Theoret. Chem. 1037, 35-48, 2014 (IF:1.371, ISI:18, S:18, GS:18, **corresponding author**)
42. T Fornaro, **M Biczysko**, S Monti, V Barone "Dispersion corrected DFT approaches for Anharmonic Vibrational Frequency Calculations: Nucleobases and their Dimers" Phys. Chem. Chem. Phys. 16, 10112-10128, 2014 (IF:3.829, ISI:29, S:36, GS:32)
43. A. Lapini, P. Fabbrizzi, M. Piccardo, M. di Donato, L. Lascialfari, P. Foggi, S. Cicchi, **M. Biczysko,** I. Carnimeo, F. Santoro, C. Cappelli, R. Righini "Ultrafast Resonant Energy Transfer in Umbelliferone-Alizarin Bichromophore" Phys. Chem. Chem. Phys. 16, 10059-10074, 2014 (IF:3.829, ISI:3, S:3, GS:3)
44. C. Puzzarini, **M. Biczysko**, J. Bloino, V. Barone "Accurate spectroscopic characterization of oxirane: a valuable route to its identification in Titan's atmosphere and the assignment of unidentified Infrared bands" The Astrophysical Journal 785, 107, 2014 (IF: 6.733, ISI:15, S:16, GS:17)
45. L. Carta, **M. Biczysko**, J. Bloino, D. Licari, V. Barone "Environmental and complexation effects on the structures and spectroscopic signatures of organic pigments relevant to cultural heritage: the case of alizarin and alizarin-Mg(II)/Al(III) complexes" Phys. Chem. Chem. Phys. 16, 2897-2911, 2014 (IF:3.829, ISI:13, S:15, GS:14, **corresponding author**)
46. C. Greco, G. Moro, L. Bertini, **M. Biczysko**, V. Barone, U. Cosentino "Computational Investigation on the Spectroscopic Properties of Thiophene Based Europium beta-Diketonate Complexes" J. Chem. Theory Comput. 10, 767-777, 2014 (IF:5.389, ISI:6, S:7, GS:8)

47. C. Puzzarini, **M. Biczysko**, V. Barone, L. Largo, I. Pena, C. Cabezas, J.L. Alonso "Accurate Characterization of the Peptide Linkage in the Gas Phase: A Joint Quantum-Chemical and Rotational Spectroscopy Study of the Glycine Dipeptide Analogue" J. Phys. Chem. Lett. 5, 534-540, 2014 (IF:6.585, ISI:22, S:27, GS:23)
48. V. Barone, **M. Biczysko**, J. Bloino, "Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation" Phys. Chem. Chem. Phys. 16, 1759-1787, 2014 (IF:3.829, ISI:110, S:141, GS:156, **Highly cited paper**)

**2013**

49. A.P. Charmet, P Stoppa, N. Tasinato, S. Giorgianni, V. Barone, **M. Biczysko**, J. Bloino, C. Cappelli, I. Carnimeo, C. Puzzarini "An integrated experimental and quantum-chemical investigation on the vibrational spectra of chlorofluoromethane" J. Chem. Phys. 139, 164302/1-16, 2013 (IF:3.164, ISI:14, S:20, GS:18)
50. I. Carnimeo, C. Puzzarini, N. Tasinato, P. Stoppa, A.P. Charmet, **M. Biczysko**, C. Cappelli, V. Barone, "Anharmonic theoretical simulations of infrared spectra of halogenated organic compounds" J. Chem. Phys. 139, 074310/1-16, 2013 (IF:3.164, ISI:34, S:42, GS:40)
51. V. Barone, **M. Biczysko**, . Bloino, F. Egidi, C. Puzzarini, "Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical" J. Chem. Phys. 139, 234303/1-14, 2013 (IF:3.164, ISI:14, S:17, GS:17, **corresponding author)**
52. C. Puzzarini, **M. Biczysko**, V. Barone, I. Pena, C. Cabezas, J.L. Alonso, "Accurate molecular structure and spectroscopic properties of nucleobases: a combined computational-microwave investigation of 2-thiouracil as a case study" Phys. Chem. Chem. Phys 15, 16965- 16975, 2013 (IF:3.829, ISI:20, S:20, GS:24)
53. N.F Aguirre, P. Villarreal, G. Delgado-Barrio, E. Posada, A. Reyes, **M. Biczysko**, A.O Mitrushchenkov, M.P. de Lara-Castells "Including nuclear quantum effects into highly correlated electronic structure calculations of weakly bound systems", J. Chem. Phys. 138, 184113/1-14, 2013 (IF:3.164, ISI:7, S:9, GS:10)
54. V. Barone, **M. Biczysko**, J. Bloino, C. Puzzarini "Accurate structure, thermodynamic and spectroscopic parameters from CC and CC/DFT schemes: the challenge of the conformational equilibrium in glycine" Phys. Chem. Chem. Phys 15, 10094-10111, 2013 (IF:3.829, ISI:43, S:52, GS:39)

55. V. Barone, **M. Biczysko**, J. Bloino, C. Puzzarini, "Characterization of the Elusive Conformers of Glycine from State-of-the-Art Structural, Thermodynamic, and Spectroscopic Computations: Theory Complements Experiment", J. Chem. Theory Comput., 9, 1533-1547, 2013 (IF:5.389, ISI:34, S:37, GS:38)
56. V. Barone, **M. Biczysko**, J. Bloino, C. Puzzarini, "Glycine conformers: a never-ending story?", Phys. Chem. Chem. Phys., 15, 1358-1363, 2013 (IF:3.829, ISI:33, S:40, GS:42)
57. G. Prampolini, F. Bellina, **M. Biczysko**, C. Cappelli, L. Carta, M. Lessi, A. Pucci, G. Ruggeri, V. Barone, Computational Design, Synthesis, and Mechanochromic Properties of New Thiophene-Based π-Conjugated Chromophores, Chemistry - A European Journal, 19, 1996-2004, 2013 (IF:5.831, ISI:17, S:29, GS:29)

**2012**

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81. V. Barone, **M. Biczysko**, M. Pavone "The role of dispersion correction to DFT for modelling

weakly bound molecular complexes in the ground and excited electronic states" - Chem. Phys. 346, 247, 2008 (IF: 1.961, ISI:62, S:65, GS:71)

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87. **M. Biczysko** and R. Tarroni "Renner–Teller interactions coupled to large spin–orbit splittings: The $BrCN^+$ case" - Chem. Phys. Lett. – 415, 223-229, 2005 (IF: 2.438, ISI:7, S:8, GS:9, **corresponding author**)
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92. **M. Biczysko** and R. Tarroni "Theoretical calculations of rovibronic energy levels and anharmonic resonances in the ground $X^2\Pi$ state of $HCP^+$ and $DCP^+$." Phys. Chem. Chem. Phys. 4, 708-715, 2002 (IF: 1.838, ISI:9, S:10, GS:11)
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94. A. Abkowicz-Bienko, **M. Biczysko** and Z. Latajka - "Solvent effect on hydrogen bonded ammonia-hydrogen halide complexes. Continuum medium versus cluster models."-Computers & Chemistry 24, 303-309, 2000 (IF: 0.9260, ISI:20, S:21, GS:23)
95. **M. Biczysko** and Z. Latajka - "Influence of water molecules on the proton position in H3N-HX (X=F,Cl,Br) complexes." - Chem. Phys. Lett. 313, 366-373, 1999 (IF: 2,269, ISI:35, S:38, GS:35)

**BOOK CHAPTERS**

1. J. Bloino, M. Biczysko "IR and Raman Spectroscopies beyond the Harmonic Approximation: The Second-Order Vibrational Perturbation Theory Formulation", in *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier, 2015, http://www.sciencedirect.com/science/article/pii/B978012409547210931X, ISBN: 978-0-12-409547-2
2. C. Puzzarini, **M. Biczysko** "Computational spectroscopy tools for molecular structure analysis" in *Structure Elucidation in Organic Chemistry: The Search for the Right Tools*, M. Cid and J. Bravo (Eds.), Willey, 2015. pp 27-64. ISBN: 978-3-527-33336-3
3. V. Barone, **M. Biczysko**, I. Carnimeo "Computational tools for Structure, Spectroscopy and Thermochemistry". in *Understanding Organometallic Reaction Mechanisms and Catalysis: Computational and Experimental Tools,* P. V. Ananikov (Ed.), Wiley-VCH, 2014, pp 249-320. ISBN 978-3-527-33562-6
4. **M. Biczysko**, J. Bloino, F. Santoro, V. Barone "Time-independent approaches to simulate electronic spectra line-shapes: from small molecules to macrosystems" in *Computational Strategies for Spectroscopy: from Small Molecules to Nano Systems*, V. Barone (Ed.) Willey, 2011, pp 361-443. ISBN: 978-0-470-47017-6
5. C. Cappelli, **M. Biczysko** "The time-independent approach to vibrational spectroscopies." in

*Computational Strategies for Spectroscopy: from Small Molecules to Nano Systems*, V. Barone (Ed.) Willey, 2011, pp 309-360. ISBN: 978-0-470-47017-6

6. V. Barone, **M. Biczysko**, P. Cimino "Interplay of stereo electronic, vibrational and environmental effects in tuning physico-chemical properties of carbon centered radicals." in *Carbon-Centered Free Radicals and Radical Cations*, M. D. E. Forbes (Ed.) John Willey & Sons, Inc., 2010, pp 105–139. ISBN: 978-0-470-39009-2

**INVITED LECTURES:**

1. **M. Biczysko** "From spectroscopic signatures to 3-D structure of protein building blocks" 10th congress of the International Society of Theoretical Chemical Physics (ISTCP), July 11-17, 2019, Tromso, Norway **invited lecture**
2. **M. Biczysko** "Computational Spectroscopy: from Astrochemistry to Biomolecules" 23rd Annual National Symposium on Computational Science and Engineering (ANSCSE23) , June 27-29, 2019, Chiang Mai University, Chiang Mai, Thailand **invited lecture**
3. **M. Biczysko**, "Molecular Systems Interacting with MIR to UV Light" Molim WG3 Workshop " Ab-Initio Modelling of Molecular Processes Under Confinement" 3-5 December 2018, Madrid, Spain **invited lecture**
4. **M. Biczysko** "Nuclear Quantum Effects in Vibrational and Electronic Spectra: the Role of Band Positions and Transition Intensities**"** Quantum International Frontiers 2018, October 17-21 2018, Changsha, Hunan Province, P.R. China **invited lecture**
5. **M. Biczysko** "Computational spectroscopy: from astrochemistry to biomolecules" 4th Polish-Taiwanese Conference "From Molecular Modeling to Nano- and Biotechnology" 29-31 August, Opole, Poland **invited lecture**
6. **M. Biczysko**, Z. Jiang, H. Zhang "Density functional theory for spectroscopy and thermochemistry" 31 Meeting of Chinese Chemical Society, May 5-8, 2018, Hangzhou, China, **invited lecture**
7. **M. Biczysko**, Z. Jiang, H. Zhang "Simulation of fully anharmonic vibrational spectra of biomolecular building blocks" AMOC 2018 Conference, April 16-19, 2018, Budapest, Hungary, **invited lecture**

8. **M. Biczysko** "Nuclear Quantum Effects On Vibrational And Electronic Spectra Line-Shapes: From Molecules To Clusters" , MOLIM-EU COST Workshop, "Multiscale Modelling - From Quantum Effects to Material Properties at the Nanoscale", Technical University of Graz in Austria, 4 to 7 February, 2018, **invited lecture**
9. **M. Biczysko** "Vibrational "fingerprints" of biomolecules building-blocks" ERCDreams Workshop "Advances in computational modelling: from isolated molecules to soft matter" November 29th to December 2nd 2017, Scuola Normale Superiore, Pisa, Italy, **invited lecture**
10. **M. Biczysko** "Anharmonic vibrational spectra: the role of band positions and intensities" The 22nd International Conference on "Horizons In Hydrogen Bond Research" 10.-14. September, 2017, Jyväskylä, Finland, **invited lecture**
11. **M. Biczysko** " "Understanding structure and function of bio-molecular systems from spectroscopic fingerprints" Conference Modeling Interactions in Biomolecules VIII (MIB VIII), Pilsen, Czech Republic, 3 - 8 September 2017, **invited lecture**
12. **M. Biczysko** "Understanding structure and function of complex soft molecular systems from spectroscopic fingerprints" DREAMS@Anacarpi Workshop, 20-22 April 2017, Anacapri (Naples) , Italy, **invited lecture**
13. **M. Biczysko** "Simulation of realistic electronic spectra band-shapes: the role of vibrational effects", 'Excited States in Complex Systems' Workshop, November, 21-23 2016, Paris France, **invited lecture**
14. **M. Biczysko** "Experimental vs computed electronic spectra: the role of vibrational effects" The 8th Molecular Quantum Mechanics, June 26 - July 1 2016, Uppsala, Sweden, **invited lecture**
15. **M. Biczysko** "Toward simulation of realistic spectral band-shapes for biomolecules" Sino-German Workshop on Biomolecular Simulations Across Scales, Shanghai, China, May 26-30, 2016, **invited lecture**
16. **M. Biczysko**, J. Bloino "Anharmonic vibrational spectra for molecular systems of increasing size and complexity" MOLIM General Meeting, Universite Paris Est - Marne la Vallee, France, 27-29 August 2015, **invited lecture**
17. **M. Biczysko** "Vibrational finger-prints and simulated spectra line-shapes: the role of band

positions and transition intensities" Advances In Computational Spectroscopy 2014, COST Action CM1002 – CODECS Final Conference, Bratislava, Slovakia 23-27 October 2014, **invited lecture**

18. **M. Biczysko**, , J. Bloino, V. Barone "Virtual multifrequency spectrometer: applications to the study of chlorophylls." International Conference on the Biophysics of Photosynthesis – BIOPH2013 – Rome, Italy, 28-30 October 2013, **invited lecture**
19. **M. Biczysko**, J. Bloino, V. Barone "Accurate Simulation and Analysis of Electronic Spectra Line-shapes by Mean of a Virtual Spectrometer" Conference "ESCE2013 - Excited States in Complex Environments", Munster, Germany, 8-11 October 2013, **invited lecture**
20. **M. Biczysko**, J. Bloino, V. Barone "Simulation of vibrational and electronic spectra with a multifrequency virtual spectrometer" Conference"Current Trends in Theoretical Chemistry VI", Krakow, Poland, 1-5 September 2013, **keynote lecture**
21. **M. Biczysko** "Integrated computational approaches for spectroscopic studies of molecular systems." CoDECS-COST Workshop, Porto, Portugal, 4-8 May, 2012, **invited lecture**.
22. V. Barone, **M. Biczysko**, J. Bloino "Computational spectroscopy of chromophoric systems in natural conditions." TheoBio - 5th symposium on Theoretical Biophysics. Madeira, Portugal, 8-12 June 2011, **invited lecture.**
23. **M. Biczysko** "Computational spectroscopy at SNS: molecular systems in natural conditions, from space to laboratory and beyond", workshop "Winter Modeling 2011", Pisa, 13-14 January 2011, **invited lecture.**
24. **M. Biczysko**, J. Bloino, V. Barone, "Non-covalent interactions in the gas phase: new insights from experimental and computational spectroscopy", "International Meeting on Atomic and Molecular Physics and Chemistry - IMAMPC 2010", Madrid, Spain, 29 June- 2 July 2010, **invited lecture.**
25. **M. Biczysko**, J. Bloino, M. Pavone, V. Barone "Toward accurate ground and excited state studies for molecular systems of biological interest", IXth International Conference on Molecular Spectroscopy, Wroclaw - Ladek Zdroj, Poland, September 12-16 2007, **invited lecture**.
26. A. Bienko, **M. Biczysko** "Theoretical modelling of proton transfer reaction in polar solvent." IHP User Group Meeting, Bologna, Italy, 28 June 2002, **invited lecture**.

27. **M. Biczysko**, P. Palmieri, Z. Latajka, R. Tarroni - "Theoretical study of potential energy surfaces for systems showing strong anharmonic effects", TAM User Group Meeting, Edinburgh, Scotland, UK, 26 March 2001, **invited lecture**.

**ORAL PRESENTATIONS:**

28. **M. Biczysko** "Computational spectroscopy for astrochemistry" The International Workshop on Astrochemistry (2019) XinjiangAstronomical Observatory, CAS; National Time Service Center, CAS May May 17-20, 2019, Xi'An China.
29. **M. Biczysko** "Molecular systems under external stimuli" The 3rd Asian Workshop on Molecular Spectroscopy March 7-9, 2019, Hefei, China.
30. **M. Biczysko**, J. Krupa, M. Wierzejewska "Theoretical studies of atmospheric molecular complexes interacting with NIR to UV light", "Quantum Effects in Small Molecular Systems: Faraday Discussion" 10-12 September 2018, Edinburgh, UK
31. **M. Biczysko**, Z. Jiang, H. Zhang "Simulation of fully anharmonic vibrational spectra of biomolecular building blocks" XXXIV European Congress on Molecular Spectroscopy - EUCMOS 2018, 19-24 August, Coimbra, Portugal
32. **M. Biczysko**, P. V. Afonine, Z. Jiang, N. W. Moriarty, Y. Xu, M. P. Waller, H. Zhang, M. Zhenga "From 3-D structure to spectroscopic properties of complex molecular systems: the Q|R route" PPES2018 "Photoinduced Processes in Embedded Systems" June 24-27, 2018, Pisa, Italy
33. **M. Biczysko**, J. Bloino "Simulation of realistic electronic spectra band-shapes: The role of vibrational effects" 255th American Chemical Society National Meeting, New Orleans, LA, US, March 18-22, 2018
34. **M. Biczysko** "Density functional theory for spectroscopy and thermochemistry" 255th American Chemical Society National Meeting, New Orleans, LA, US, March 18-22, 2018
35. **M. Biczysko**, J. Bloino "Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism, and Raman Optical Activity", WATOC 2017 - 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany, August 27-September 1 2017
36. **M. Biczysko**, J. Bloino, "Fully anharmonic IR, Raman, VCD and ROA spectra from

GVPT2", 33rd European Congress on Molecular Spectroscopy (EUCMOS 2016), University of Szeged, Hungary, 30 July - 4 August 2016

37. **M. Biczysko** Simulation of Realistic Electronic Spectra Band-shapes of Chromophores Relevant for Material Science" The 9th International Conference on Computational Nanoscience and New Energy Materials (CNNEM-2016), Shanghai, PR. China, June 22-26, 2016
38. **M. Biczysko**, J. Bloino "Simulation of realistic electronic spectra band-shapes of chromophoric systems relevant for solar light harvesting" 251st American Chemical Society National Meeting & Exposition, "Computers in Chemistry" San Diego, California, March 13-17 2016.
39. **M. Biczysko** "Simulation of electronic spectra line-shapes of chlorophylls in different environmental conditions", The International Chemical Congress of Pacific Basin Societies 2015: Pacifichem 2015, Honolulu, Hawaii, USA December, 15 - 20, 2015
40. **M. Biczysko,** T. Fornaro, J. Bloino, "Spectroscopic features of molecular aggregates from anharmonic computations" The International Chemical Congress of Pacific Basin Societies 2015: Pacifichem 2015, Honolulu, Hawaii, USA December, 15 - 20, 2015
41. **M. Biczysko,** J. Bloino "Theoretical Vibrational Finger-Prints for Medium-Sized Molecules: The Role of Band Position and Intensities" The 23rd International Conference on High Resolution Molecular Spectroscopy, Bologna, Italy, September 2-6, 2014, **oral**
42. **M. Biczysko**, J. Bloino, V. Barone "Multifrequency Virtual Spectrometer for Astrochemistry Applications" 248rd American Chemical Society National Meeting & Exposition, San Francisco, CA, August 10-14, 2014, **oral**
43. V. Barone, **M. Biczysko**, J. Bloino, I. Carnimeo, T. Fornaro "Anharmonic IR Spectra of Biomolecules: Nucleobases and their Oligomers" 69th OSU International Symposium on Molecular Spectroscopy Champaign-Urbana, Illinois, US, June 16-20, 2014, **oral**
44. V. Barone, **M. Biczysko**, J. Bloino, I. Carnimeo, C. Puzzarini "Accurate Anharmonic IR Spectra from Integrated CC/DFT Approach" 69th OSU International Symposium on Molecular Spectroscopy Champaign-Urbana, Illinois, US, June 16-20, 2014, **oral**
45. **M. Biczysko**, J. Bloino, V. Barone "Toward computational spectroscopy studies for large molecular systems" 68th OSU International Symposium on Molecular Spectroscopy Columbus, Ohio, US, June 17-21, 2013, **oral**

46. **M. Biczysko**, J. Bloino, V. Barone ““Simulation of High Resolution Vibrational and Electronic Spectra with a Multifrequency Virtual Spectrometer” 68th OSU International Symposium on Molecular Spectroscopy, Columbus, Ohio, US, June 17-21, 2013, **oral**
47. **M. Biczysko**, J. Bloino, V. Barone “Simulation of optical spectra line-shapes for biomolecules in natural environmental conditions.” OWLS-Optics Within Life Sciences Genoa, Italy, 4-6 July 2012, **oral**.
48. **M. Biczysko**, J. Bloino, V. Barone “Simulation of vibrational and electronic spectra line-shapes for chromophoric systems relevant for renewable energy sources.” 243rd American Chemical Society National Meeting & Exposition. San Diego, CA, March 25-29 2012, **oral**.
49. **M. Biczysko**, J. Bloino, V. Barone “Simulation of optical spectra line-shapes for molecular systems in natural conditions, form space to laboratory and beyond.” TheTIS 2011 "Theoretical Tools for In Silico Spectroscopy" Codecs-COST Action CM1002 Meeting. Paris, France, 13-15 April 2011, **oral**.
50. **M. Biczysko**, J. Bloino, V. Barone “Simulation of optical spectra line-shapes for chromophoric systems in natural conditions.” Modelling of biologically-inspired photoactive systems. Marseille, France, 30-31 March, 1 April 2011, **oral**.
51. **M. Biczysko**, J. Bloino, M. Borkowska-Panek, V. Barone “Toward an understanding of chlorophylls: Simulation of the coordination and vibrational effects in the UV-vis spectra.” Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011. Santiago de Compostela, Spain, 17-22 July 2011**, oral**.
52. **M. Biczysko** “Computational spectroscopy as a tool to interpret experimental results: from small molecules in the gas phase to large systems in condensed phases”, EUCMOS 2010 - 30th European Congress of Molecular Spectroscopy, Firenze, 29 August- 3 September 2010, **oral.**
53. **M. Biczysko,** J. Bloino, M. Pavone, V. Barone “Integrated approach to compute optical spectra for molecular systems of biological interest”, Winter Modeling 2008, Pisa, Italia, 19 December 2008, **oral.**
54. **M. Biczysko**, J. Bloino, M. Pavone, V. Barone “Integrated computational approaches for ground and excited state studies for molecular systems of biological interest ”, Current Trends in Theoretical Chemistry V, Krakow, Poland, 6-10 July 2008, **oral.**
55. **M. Biczysko**, A.J.C. Varandas ”Accurate ab initio calculation of reaction steps for nitrogen

hydrogenation leading to ammonia" Workshop "Predicting Catalysis: Understanding Ammonia Production from First Principles", Leiden, Olanda, 21-23 June 2006, **oral**.

56. **M. Biczysko**, L. A. Poveda and A. J. C. Varandas "Single-sheeted double many-body expansion potential energy surface for $N_2H_2$ ($^1A$) from accurate MRCI calculations." EC RTN Midterm Meeting, Innsbruck, Austria, 24-26 February 2005, **oral**.
57. **M. Biczysko**, L. A. Poveda, V. C. Mota and A. J. C. Varandas "Toward a global potential energy surface for $N_2H_2$", EC RTN Meeting, Coimbra, Portugal, 23-25 April 2004, **oral.**
58. **M. Biczysko**, "Vibrational calculations for anharmonic systems", Theonet II Meeting, Cambridge, UK, 12-15 September 2002, **oral.**
59. **M. Biczysko**, P. Palmieri, R. Tarroni "Rovibronic levels for systems showing the Renner-Teller effect and large spin-orbit coupling", Theonet II Meeting, Helsinki, Finland, 1-2 September 2001, **oral**.
60. **M. Biczysko**, P. Palmieri, R. Tarroni "Rovibronic levels for $HBS^+$, a radical cation showing the Renner-Teller effect and large spin-orbit coupling", Gruppo Nazionale Cofinanziamento MURST ,II Riunione Scientifica delle Unita di Ricerca, , Roma, Italy, Jun. 2001 **oral.**

## INVITED SEMINARS

1. **M. Biczysko** ""Simulation of vibrational and electronic spectra with a multifrequency virtual spectrometer: accuracy and interpretation." Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland, 22 December 2014.
2. **M. Biczysko** "Toward reliable line-shapes for the electronic spectra of large molecular systems", Wroclaw Centre for Networking and Supercomputing, Wroclaw, Poland, 22 September 2010
3. **M. Biczysko "**Toward reliable line-shapes for the electronic spectra of large molecular systems", Gorlaeus Laboratories, Universiteit Leiden, Netherlands, 10 June 2010
4. **M. Biczysko** "Vibrationally resolved electronic spectra in Gaussian 09", Institute of Physical and Theoretical Chemistry, Department of Chemistry of the Wroclaw University of Technology, Wroclaw, Poland, September 2009

## TEACHING

1. **Modeling of Soft Molecular Systems**, Master Course at Shanghai University (2016-2020)
2. **Professional English,** Undergraduate Course at Shanghai University (2018-2019)

3. **Advances in Physics,** Undergraduate Course at Shanghai University (2018-2019)
4. **Quantum statistics,** Master Course at Shanghai University (2016-2017)
5. **Excited states and photochemistry** The European and Erasmus Mundus Master in Theoretical Chemistry and Computational Modelling (TCCM), September 5-30, 2016 Porto, Portugal
6. **Vibrational Spectra and Thermochemistry**, Smart (Space-time Multiscale Approaches for Research and Technology) Winter School, Scuola Normale Superiore, January 25-29, 2016, Pisa, Italy
7. **Simulation of electronic and vibrational spectra line-shapes** - CoDECS Summer School on Theoretical Spectroscopy 2013, 26-30 August, 2013, Geneva, Switzerland
8. **Molecular Spectroscopy** (series of lectures on Computational Spectroscopy) 2013, Scuola Normale Superiore, Pisa, Italy
9. **Computational Modeling of Bio- and Nano-systems** (series of lectures + exercises), 2012-2014, Scuola Normale Superiore, Pisa, Italy
10. **Frontiers in Chemistry** (introductory lectures), 2011-2012**,** Scuola Normale Superiore, Pisa, Italy
11. **Modeling of complex systems,** 2010, The European and Erasmus Mundus Master in Theoretical Chemistry and Computational Modeling, Porto, Portugal
12. **Socrates-Erasmus program**, 2008-2010, student project tutoring (P. Kus, S. Bakowski, P. Panek, M. Borkowska-Panek, M. Dargiewicz, D. Michalski) University di Wroclaw, Poland/ Università Federico II, Naples, Italy
13. **Computational Chemistry** (support of didactical activity) 2006-2010, Università Federico II, Naples, Italy
14. **Elements of physical and quantum chemistry,** 1996- 1999, University of Wroclaw, Poland
15. **Quantum chemistry,** 1995-1999 , University of Wroclaw, Poland
16. **Statistical thermodynamics,** 1994-1999, University of Wroclaw, Poland

## THESIS SUPERVISION

1. MSc Thesis: Zhenlong Gong “Effective computational models for protein science” Shanghai University, to be graduated July 2020, co-supervisor
2. MSc Thesis: Mingzhu Sheng “Structural and spectroscopic studies of weak interactions in bio-molecules” Shanghai University, to be graduated July 2020, co-supervisor

3. MSc Thesis: Chong Shu "Accurate determination of structural and energetic properties of peptides building-blocks" Shanghai University, to be graduated July 2020, co-supervisor
4. MSc Thesis: Xinxing Li "Simulation of fluorescent dyes optical properties" Shanghai University, to be graduated July 2020
5. MSc Thesis: Hongli Zhang "Understanding the structure-function relationships by simulating and interpreting spectroscopic outcomes" Shanghai University, graduated July 2019
6. MSc Thesis: Zhongming Jiang "Accurate determination of energies and molecular structures for isolated amino acids and small peptides mimicking protein local arrangements" Shanghai University, graduated July 2018
7. PhD Thesis. Teresa Fornaro "Spectroscopic Studies of Molecular Systems Relevant in Astrobiology" Scuola Normale Superiore, Pisa, January 2016, co-supervisor
8. PhD Thesis: Luciano Carta "Interpretation and prediction of optical properties of medium-to-large systems by computational approaches", Scuola Normale Superiore, Pisa, March 2014, co-supervisor
9. MSc Thesis: Pawel Panek "Theoretical studies of vibrational spectra for model molecular systems" University of Wroclaw, 2010, co-supervisor
10. MSc Thesis: Monika Borkowska-Panek "Theoretical studies of spectroscopic properties of chlorophyll-a" University of Wroclaw, 2010, co-supervisor
11. MSc Thesis: Monika Dargewicz "DFT study on electron-driven proton-transfer processes in DNA complexes" University of Wroclaw, 2010, co-supervisor

**CONGRESS ORGANISING**

1. "Elsevier Chemistry Connect China Tour – Chemistry Advancing Health" 25 March 2019, Shanghai, China, Chair of Local Organizing Committee
2. International Astro-Spectroscopy Symposium, 20 November 2018, Shanghai, China, Chair of Local Organizing Committee
3. International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC), 19-22 June 2017, Torun, Poland; Member of International Scientific Committee

4. Smart (Space-time Multiscale Approaches for Research and Technology) Winter School, Scuola Normale Superiore, January 25-29, 2016, Member of International Organizing and Scientific Committee
5. Winter Modeling: Special Edition “In the frameworks of DREAMS”, Scuola Normale Superiore, December 1-2, 2014, Pisa, Italy, co-Chair
6. The 23rd International Conference on High Resolution Molecular Spectroscopy, Bologna, Italy, September 2-6, 2014, member of local organizing committee.
7. “CoDECS Summer School on Theoretical Spectroscopy 2013”, 26-30 August, 2013, Geneva, Switzerland, member of scientific and organizing committees.
8. IMAMPC 2013 - International Meeting on Atomic and Molecular Physics and Chemistry, 02-05 July 2013, Lille, France, member of the scientific committee.
9. “Convergent Distributed Environment for Computational Spectroscopy” CoDECS 2013 Workshop, April 18-22, 2013, San Lorenzo de El Escorial, Madrid (Spain), member of the scientific and organizing committees.
10. International Conference “Theory, Experiments and Modelling of Chemical Processes, Dynamics and Molecular Interactions”, 29 November 29 2012, Bologna, Italy, member of the organizing committee
11. IMAMPC 2012 - International Meeting on Atomic and Molecular Physics and Chemistry, Scuola Normale Superiore, 12-14 September 2012, Pisa, Italy, member of scientific and organizing committees
12. "Winter Modeling: Special Edition" CMST Action CM1002 - CODECS Workshop, Scuola Normale Superiore, November 9, 2012, Pisa, Italy, member of the organizing committee
13. "Holistic Computational Spectroscopy: innovative concepts, modern tools, strategic vision and challenges" CMST Action CM1002 - CODECS Workshop, Scuola Normale Superiore, November 16-18, 2011, Pisa, Italy, member of scientific and organizing committees
14. Workshop “Inauguration of International Year of Chemistry”, Scuola Nazionale Superiore 11 February 2011, Pisa, Italia, member of the organizing committee
15. Workshop “Winter Modeling 2010”, Scuola Nazionale Superiore, 26 February 2010, Pisa, Italia, member of the organizing committee.

**GRANTS/PROJECTS**

1. SHU-Global grant for High-end International Academic Conference, Quantum International Frontiers, 2019/01-2019/12, total amount 150’000 yuan, in research, MB is project host
2. National Natural Science Foundation of China, 31870738, Quantum Refinement: the next generation method for bio-crystallography and cryo-EM, 2019/01 - 2022/12, total amount about 450’000 yuan, in research, MB is a project member.
3. National Natural Science Foundation of China Major Research Program - Cultivation Project 91641128, Molecular Simulation Study on Low - polluting Combustion Reaction Mechanism of Aero - Engine Hydrocarbon Fuel, 2017/01 - 2019/12, Total amount of about 700,000 yuan. MB is a project member.
4. European Cooperation in Science and Technology (COST), COST Action CM1405, MOLecules In Motion, 2015/03-2019/03, 400 kEUR. MB is Managment Committee Member
5. European Cooperation in Science and Technology (COST), COST Action CM1002: COnverged Distributed Environment for Computational Spectroscopy (CODECS, www.idea.sns.it/CODECS), 2010-2014. MB actively participated to the preparation of grant proposal, and has been responsible during the project for the scientific and administrative organization, budget planning and reporting on behalf of CoDECS Action Chair Prof. Vincenzo Barone and CoDECS Management Committee.
6. European Union's Seventh Framework Programme (FP7/2007-2013) Grant Agreement No ERC-2012-AdG-320951-DREAMS “Development of a Research Environment for Advanced Modelling of Soft matter”, Principal Investigator Prof. Vincenzo Barone, (2013-2018), total budget about 2’000’000 EUR (http://dreamserc.sns.it/). MB actively participated to the project proposal preparation and have been responsible for the scientific reporting.
7. Grant within HPC-Europa2. The HPC-Europa2 project is funded by the European Commission - DG Research in the Seventh Framework Programme under grant agreement n° 228398 and aims on sharing Pan-European Research Infrastructure on High Performance Computing and foster international collaboration. HPC-Europa2 research grant for the project “Computational studies on spectroscopic properties of polysulfanes and diallyltetrasulfide” assigned in 2012 to Dr. Krzysztof Mierzwicki. MB acted as a grant coordinator and scientific host.
8. HPC-Europa2 research grant for the project “Spectroscopic Properties of Chlorophyll-a - Theoretical Study”, assigned in 2011 to Ms Monika Borkowska_Panek. MB acted as a grant coordinator and scientific host

9. PON 01_01078 “Identification of biomarkers and development of diagnostic and therapeutic methods in the field of oncology and vascular biology”. MB has been a project member.
10. FIRB Futuro in Ricerca 2010, 3-year (2010-2013) National Research Grant for the project “Studies of energy and charge transfer in new multichromophoric systems of increasing complexity: toward “intelligent” materials for organic photovoltaics”, national Coordinator: Dr. MariaAngela Di Donato, total grant 770’000 EUR, MB actively participated to the project proposal preparation and has been a project member.
11. PRIN 2009 ``Molecular Spectroscopy for Atmospherical and Astrochemical Research: Experiment, Theory and Applications" – MB has been a project member.
12. PRIN08 "Theory, Experiments And Modelling Of Chemical Processes, Dynamics And Molecular Interactions", a national 2-year research grant, National Coordinator: Prof. Walther Caminati, Pisa research Unit: “Application and development of integrated computational approaches for studies of spectroscopic properties and dynamics of molecules and molecular aggregates.” Local Coordinator: Prof. Ivo Cacelli, local budget about 60’000 EUR. MB has actively participated to the project proposal preparation and has been responsible for the coordination of joint research with Florence Research Unit (Dr. Maurizio Becucci, LENS, the European Laboratory for Non-linear Spectroscopy).
13. Research grant at computational center CINECA, Casalechio di Reno (Bo), within the European MINOS project. MB received a grant for the research project “Calculations of highly accurate rovibronic levels for systems showing non-adiabatic interactions”, 2 month initial stay at CINECA supercomputer center along with generous computer time for next 3 years.
14. Research grant from University of Lubljana (Slovenia) for 3-months stay at the Laboratory of Prof. Dusan Hadzi to work on "Modulation of the phenol hydrogen bonding propensity of phenol by Pi-bonding: Possible role of tyrosine in receptor triggering."