Heribert Reis

Scientific Technical Personnel
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Education and qualifications

1988: Diploma in Chemistry, Department of Physical Chemistry – Johannes-Gutenberg University of Mainz, Germany.

1995: PhD in Chemistry, Department of Physical Chemistry – University of Mainz, Germany. Supervisor: Prof. Wolfram Baumann.

Appointments

1995 - 1997

Scientifiic Employee, Department of Physical Chemistry, Research Associate, Department of Food Technology, Technological Educational Institution of Athens

03/1997 – 05/2000

Postdoc at Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation

06/2000 - 08/2005

Participation in several projects of the National Hellenic Research Foundation

09/2005 - present

Scientific Technical Personnel, Institute of Biology, Medicinal Chemistry and Biotechnology, National Hellenic Research Foundation

06/2012 – 05/2013

Visiting researcher at the Interdisciplinary Center for Nanotoxicity, Jackson, Mississippi, USA

04/05/2014 – 15/06/2015

Invited Lecturer at the Mathematical and Natural Science Faculty of the Jan dlugosz University in Czestochowa, Poland.

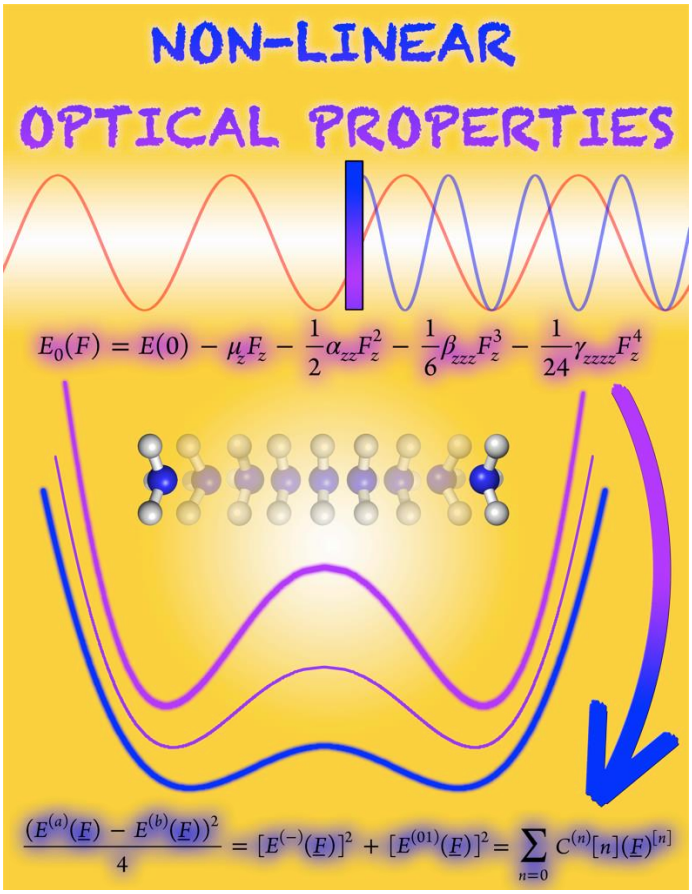
09/2014 – 10/2015

Invited external expert at the Matej Bel University, Banska Bystrica, Slovakia

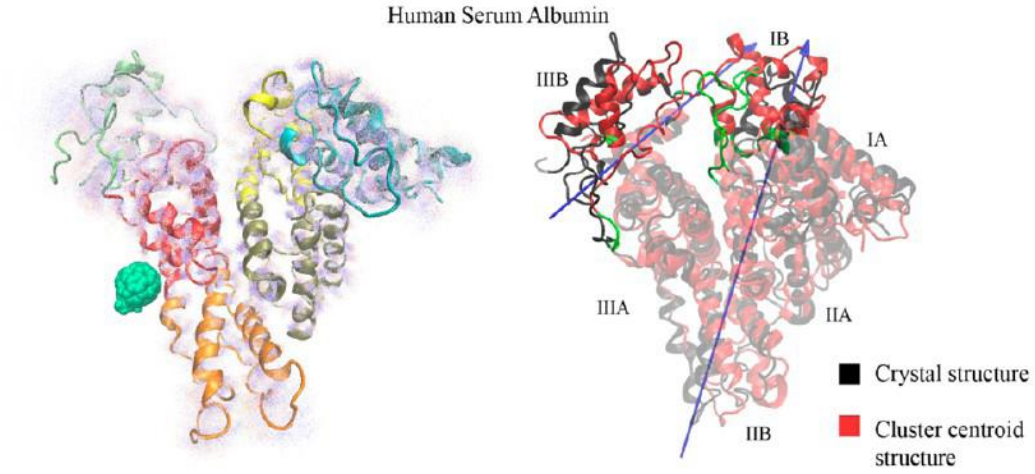
Research interests

1. Experimental determination of dipole moments and polarizabilities in ground and excited electronic states

2. Theoretical prediction of linear and nonlinear optical (NLO) properties of molecules, nanomaterials and condensed phases. In an effort to develop efficient methods to compute the NLO properties of materials, we have developed and implemented an approach for the computation of the NLO properties of molecular crystals, liquids and polymers. We are trying to extend these methods to novel materials, like nanomaterials, which show very promising NLO properties. I'm also working on developing methods for the accurate determination of the vibrational contributions to NLO properties, with special emphasis on molecules exhibiting large-amplitude motions, such as the umbrella motion in ammonia.



3. Application of accurate *ab-initio* methods to large-scale problems involving bioactive compounds. Examples include the application of the effective fragment potential (EFG) approach to the elucidation of the binding mechanism of renin, or the use of the fragment molecular method (FMO) to the investigation of the interaction between fullerenes and human serum albumin.



Foreign Languages

-English, Spanish, Portuguese, Greek

Current collaborations (outside NHRF)

International

1. Dr. Josep Maria Luis, Department of Chemistry, University of Gironal, Spain.
2. Prof. Claude Millot, University of Lorraine, Nancy, France.
3. Prof. Bernard Kirtman, Departmant of Chemistry and Biochemistry, University of California, Santa Barbara, USA
4. Dr. Robert Zalesny, Institute of Physical and Theoretical Chemistry, Wrocalw University of Technology, Poland
5. Dr. Miroslav Medved, Department of Chemistry, Faculty of Natural Sciences, Matej Bel University, Slovakia
6. Dr. Bakthiyor Rasulev, North Dakota State University, USA
7. Prof. Jerzy Lesczynski, Jackson State University, USA
8. Prof. Sakir Erkoc, Physics Department, Middle East Technical University, Ankara, Turkey

9. Prof. Patricia Calaminici, CINVESTAV, Mexiko
10. Prof. Andreas Koester, CINVESTAV, Mexiko
11. Prof. Janos Angyan, Directeur de Recherches u CNRS, Universite de Lorraine, France.
12. Prof. Christof Hättig, TheoChem, Ruhr-University Bochum.
13. Prof. Robert W. Munn, Department of Chemistry, University of Manchester
14. Dr. David Lauvergnat, Laboratory of Chemical Physics, CNRS and University of Paris-Sud, France,

Publications

Publications in Peer Reviewed Scientific Journals

1) S.V. Rodrigues, A.K. Maiti, H. Reis, W. Baumann, “Electrooptical Emission Measurements on a Nonconjugated Bichromophoric Donor-Acceptor Molecule”, MOLECULAR PHYSICS 1992, Vol 75, pp 953-960.
2) W. Baumann, Z. Nagy, H. Reis, N. Detzer,“Electric-Field-Induced Anisotropy Spectra”, CHEMICAL PHYSICS LETTERS 1994, Vol 224, pp 517-524.
3) N.A. Nemkovich, W. Baumann, H. Reis, N. Detzer,“Dipole-Moments of Aminophthalimides Determined by Modified Electrooptical Absorption and Emission Measurements”, JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY 1995, Vol 89, pp 127-133.
4) N.A. Nemkovich, W. Baumann, H. Reis, Y.V. Zvinevich, “Electrooptical and Laser Spectrofluorometry Study of Coumarin-7 and Coumarin-30 - Evidence for the Existence of the Close-Lying Electronic States and Conformers”, JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY 1997, Vol 109, pp 287-292.
5) N.A. Nemkovich, H. Reis, W. Baumann, “Ground and Excited-State Dipole-Moments of Coumarin Laser-Dyes - Investigation by Electrooptical Absorption and Emission Methods”, JOURNAL OF LUMINESCENCE 1997, Vol 71, pp 255-263.
6) C. Carvalho, I. Brinn, W. Baumann, H. Reis, Z. Nagy, “Excited-State Acidity of Bifunctional Compounds .5. 5-(2-Hydroxyphenyl)-3-Phenyl-1,2,4-Oxadiazole and 3-(2-Hydroxyphenyl)-5-Phenyl-1,2,4-Oxadiazole”, JOURNAL OF THE CHEMICAL SOCIETY-FARADAY TRANSACTIONS 1997, Vol 93, pp 3325-3329.
7) H. Reis, W. Baumann,“Influence of Rotational Diffusion on the Electric-Field-Induced Effect on the Fluorescence-Spectrum of Diluted Solutions .1. Theory and Numerical Simulations”, CHEMICAL PHYSICS 1997, Vol 214, pp 383-407.
8) K. Nishiyama, T. Honda, H. Reis, U. Mueller, K. Muellen, W. Baumann, T. Okada, “Electronic-Structures of 9,10-Anthrylene Dimers and Trimers in Solution - Formation of Charge Separation States Depending on Alkyl Substituent Groups”, JOURNAL OF PHYSICAL CHEMISTRY A 1998, Vol 102, pp 2934-2943.

9) H. Reis, S. Raptis, M.G. Papadopoulos, R.H.C. Janssen, D.N. Theodorou, R.W. Munn, "Calculation of Macroscopic First-Order and 3rd-Order Optical Susceptibilities for the Benzene Crystal", THEORETICAL CHEMISTRY ACCOUNTS 1998, Vol 99, pp 384-390.
10) H. Reis, M.G. Papadopoulos, R.W. Munn, "Calculation of Macroscopic First-Order, 2nd-Order, and 3rd-Order Optical Susceptibilities for the Urea Crystal", JOURNAL OF CHEMICAL PHYSICS 1998, Vol 109, pp 6828-6838.
11) N.A. Nemkovich, W. Baumann, H. Reis, Y.V. Zvinevich, A.N. Rubinov, "Dipole-Moments of Laser Coumarins in the Ground and Excited Electronic States", OPTICS AND SPECTROSCOPY 1999, Vol 87, pp 735-741.
12) R. Wortmann, S. Lebus, H. Reis, A. Grabowska, K. Kownacki, S. Jarosz, "Spectral and Electrooptical Absorption and Emission Studies on Internally Hydrogen-Bonded Benzoxazole Double Derivatives - 2,5-bis(Benzoxazolyl)Hydroquinone (Bbhq) and 3,6-is(Benzoxazolyl)Pyrocatechol (Bbpc) - Single Versus Double Proton-Transfer in the Excited Bbpc Revisited", CHEMICAL PHYSICS 1999, Vol 243, pp 295-304.
13) H. Reis, M.G. Papadopoulos, "Nonlinear-Optical Properties of the Rhombic B-4-Cluster", JOURNAL OF COMPUTATIONAL CHEMISTRY 1999, Vol 20, pp 679-687.
14) H. Reis, M.G. Papadopoulos, I. Boustani, "DFT calculations of Static Dipole Polarizabilities and hyperpolarizabilities for the Boron Clusters Bn (n=3-8,10)", INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 2000, Vol 78, pp 131-135.
15) H. Reis, M.G. Papadopoulos, C. Haettig, J.G. Angyan, R.W. Munn "Distributed First and 2nd-Order Hyperpolarizabilities - An Improved Calculation of Nonlinear-Optical Susceptibilities of Molecular Crystals", JOURNAL OF CHEMICAL PHYSICS 2000, Vol 112, pp 6161-6172.
16) H. Reis, M.G. Papadopoulos, P. Calaminici, K. Jug, A. Köster, "Calculation of macroscopic linear and nonlinear optical susceptibilities for the naphthalene, anthracene and meta-nitroaniline crystals", CHEMICAL PHYSICS 2000, Vol 261, pp 359-371.
17) H. Reis, S.G. Raptis, M.G. Papadopoulos, "Electrostatic calculation of linear and nonlinear optical properties of ice Ih, II, IX and VIII.", CHEMICAL PHYSICS 2001, Vol. 263, 301-16.
18) Detsi, E. Gavrielatos, M.A. Adam, O. Igglessi-Markopoulou, J. Markopoulos, M. Theologitis, H. Reis and M.G. Papadopoulos, "Synthesis of N-Urethane-Protected Gamma-Amino-Functionalized Butenoates and Tautomeric Studies by Means of NMR, X-Ray Crystallography and Ab-Initio Calculations", EUROPEAN JOURNAL OF ORGANIC CHEMISTRY 2001, pp 4337-4342
19) H. Reis, M.G. Papadopoulos, D.N. Theodorou, "Calculation of Refractive-Indexes and 3rd-Harmonic Generation Susceptibilities of Liquid Benzene and Water - Comparison of Continuum and Discrete Local-Field Theories", JOURNAL OF CHEMICAL PHYSICS 2001, Vol 114, pp 876-881.
20) H Reis, S. Raptis, M.G. Papadopoulos, "Comparison of the non-linear optical properties of a dimethylaminostilbene derivative containing a molybdenum mononitrosyl redox centre and of p,p'-dimethylaminonitrostilbene calculated by ab-initio methods", PHYSICAL CHEMISTRY CHEMICAL PHYSICS 2001, Vol. 3, 3901-3905
21) R.W. Munn, M.G. Papadopoulos, H. Reis, "Local fields and distributed response: Electric susceptibility calculations for molecular materials", POLISH JOURNAL OF CHEMISTRY 2002, Vol. 76, 155-165.

22) H Reis, M.G. Papadopoulos, “Calculation of the first hyperpolarizabilities of the neutral and the cationic form of a donor-acceptor molecule containing octamethylferrocene”, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 2003, Vol. 5, 1190-1192.
23) H. Reis, M. G. Papadopoulos, A. Avramopoulos, “Calculation of the microscopic and macroscopic linear and nonlinear optical properties of acetonitrile: I. Accurate molecular properties in the gas phase and susceptibilities of the liquid in Onsager's reaction-field model”, JOURNAL OF PHYSICAL CHEMISTRY A 107, 3907-3917, 2003.
24) R. Wortmann, S. Lebus-Henn, H. Reis, M. G. Papadopoulos, “Off-diagonal second-order polarizability of N,N '-dihexyl-1,3-diamino-4,6-dinitrobenzene”, JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 633 (2-3): 217-226, 2003
25) H Reis, M. Makowska-Janusika, M. G. Papadopoulos, “Nonlinear optical susceptibilities of poled guest-host systems: A computational approach” JOURNAL OF PHYSICAL CHEMISTRY B 108 (26): 8931-8940, 2004
26) Avramopoulos A, Reis H, Li JB, et al. “The dipole moment, polarizabilities, and first hyperpolarizabilities of HArF. A computational and comparative study” JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 126 (19): 6179-6184, 2004
27) Makowska-Janusik M, Reis H, Papadopoulos MG, et al.Molecular dynamics simulations of electric field poled nonlinear optical chromophores incorporated in a polymer matrix JOURNAL OF PHYSICAL CHEMISTRY B 108 (2): 588-596, 2004
28) Papadopoulos MG, Reis H, Avramopoulos A, et al. A comparative study of the dipole polarizability of some Zn clusters J PHYS CHEM B 109 (40): 18822-18830 OCT 13 2005
29) Makowska-Janusik M, Reis H, Papadopoulos MG, Economou IG Peculiarities of electric field alignment of nonlinear optical chromophores incorporated into thin film polymer matrix. THEORETICAL CHEMISTRY ACCOUNTS114 (1-3): 153-158 SEP 2005
30) Souli C, Avlonitis N, Calogeropoulou T, Tsotinis A, Maksay G, Biro T, Politi A, Mavromoustakos T, Makriyannis A, Reis H, Papadopoulos M Novel 17 beta-substituted conformationally constrained neurosteroids that modulate GABA(A) receptors JOURNAL OF MEDICINAL CHEMISTRY 48 (16): 5203-5214 AUG 11 2005
31) H. Reis, A. Grzybowski, and M. G. Papadopoulos Computer Simulation of the Linear and Nonlinear Optical Susceptibilities of p-Nitroaniline in Cyclohexane, 1,4-Dioxane, and Tetrahydrofuran in Quadrupolar Approximation. I. Molecular Polarizabilities and Hyperpolarizabilities JOURNAL OF PHYSICAL CHEMISTRY A 109, 9911, 2005
32) Munn, RW; Papadopoulos, MG; Reis, H Local fields and distributed response: Electric susceptibility calculations for molecular materials POLISH JOURNAL OF CHEMISTRY 76 (2002) 155-165
33) Alparone, A; Reis, H; Papadopoulos, MG Theoretical investigation of the (hyper) polarizabilities of pyrrole homologues C4H4XH (X = N, P, As, Sb, Bi). A coupled-cluster and density functional theory study JOURNAL OF PHYSICAL CHEMISTRY A 110 (2006) 5909-5918
34) Papadopoulos, MG; Reis, H; Avramopoulos, A; Erkoc, S; Amirouche, L Polarizabilities and second hyperpolarizabilities of ZnmCdn clusters MOLECULAR PHYSICS 104 (2006) 2027-2036
35) Reis, H; Papadopoulos, MG; Grzybowski, A Computer simulation of the linear and nonlinear optical susceptibilities of p-nitroaniline in cyclohexane, 1,4-dioxane, and tetrahydrofuran in

quadrupolar approximation. II. Local field effects and optical susceptibilitities JOURNAL OF PHYSICAL CHEMISTRY B 125 (2006) 18537-18552

36) Reis, H Problems in the comparison of theoretical and experimental hyperpolarizabilities revisited JOURNAL OF CHEMICAL PHYSICS 125 (2006) 014506
37) Avramopoulos, A; Papadopoulos, MG; Reis, H Calculation of the microscopic and macroscopic linear and nonlinear optical properties of liquid acetonitrile. II. Local fields and linear and nonlinear susceptibilities in quadrupolar approximation JOURNAL OF PHYSICAL CHEMISTRY B 111 (2007) 2546-2553.
38) Avramopoulos, A; Serrano-Andres, L; Li, JB; Reis, H; Papadopoulos, MG Linear and nonlinear optical properties of some organoxenon derivatives JOURNAL OF CHEMICAL PHYSICS 127 (2009) 214102
39) Durdagi, S; Reis, H; Papadopoulos, MG; Mavromoustakos, T Comparative molecular dynamics simulations of the potent synthetic classical cannabinoid ligand AMG3 in solution and at binding site of the CB1 and CB2 receptors BIOORGANIC & MEDICINAL CHEMISTRY 16 (2008) 7377-7388
40) Loboda, O; Zalesny, R; Avramopoulos, A; Luis, JM; Kirtman, B; Tagmatarchis, N; Reis, H; Papadopoulos, MG Linear and Nonlinear Optical Properties of [60]Fullerene Derivatives JOURNAL OF PHYSICAL CHEMISTRY A 113 (2009) 1159-1170
41) Luis, JM; Reis, H; Papadopoulos, M; Kirtman, B Treatment of nonlinear optical properties due to large amplitude anharmonic vibrational motions: Umbrella motion in NH3 JOURNAL OF CHEMICAL PHYSICS 131 (2009) 034116
42) Reis, H; Oloboda, O., Avramopoulos, A.; Papadopoulos, M.G.; Kirtman, B.; Luis, J.M.; Zalesny, R, Electronic and vibrational linear and non-linear polarizabilities of Li@C60 and [Li@C60]+ Journal of Computational Chemistry 32 (2011) 908
43) Fotakis, D. Christodouleas, P. Zoumpoulakis, E. Kritsi, N.-P. Benetis, T. Mavromoustakos, H. Reis, A. Gili, M.G. Papadopoulos, M. Zervou, Comparative Biophysical Studies of Sartan Class Drug Molecules Losartan and Candesartan (CV-11974) with Membrane Bilayers. J. Phys. Chem. B 115, 6180-6192 (2011).
44) Skwara, R.W.Gora, R. Zalesny, P. Lopkowski, W. Bartkowiak, H. Reis, MG Papadopoulos, JM Luis, B. Kirtman, Electronic structure, Bonding, Spectra and Linear and Nonlinear Optical Properties of Ti@C28, J. Phys. Chem. A 115, 10370-10381 (2011).
45) B. Kirtman, V. Lacivita, R. Dovesi, H. Reis, Electric field polarization in conventional density-functional theory: From quasilinear to two-dimensional and three-dimensional extended systems, J. Chem. Phys. 135, 154101 (2011).
46) B. Skwara, O.Loboda, A. Avramopoulos, JM Luis, H. Reis, MG Papadopoulos, Electronic Contributions to Linear and Nonlinear Optical Properties in Fullerene-based Molecular Materials, AIP Conference Proceedings 1504, 406-413 (2012).
47) Avramopoulos, H.Reis, MG Papadopoulos, The Effect of the Vibrational Contributions to the Non-Linear Optical Properties of Small and Medium-sized Molecules, AIP Conference Proceedings 1504, 414-423 (2012).
48) JM Luis, H Reis, MG Papadopoulos, B Kirtman, Nonlinear optical properties and large amplitude anharmonic vibrational motions, AIP Conference Proceedings 1504, 607-610 (2012).

49) H Reis, JM Luis, Prediction of the Linear and Nonlinear Optical susceptibilities of 3-methyl-4-nitropyridine-N-oxide (POM) and m-nitroaniline (mNA) Crystals with Account of Electronic and Molecular Vibrational Contributions, AIP Conference Proceedings 1504, 643-646 (2012).
50) G. Leonis, Z. Czyznikowska, G. Megariotis, H. Reis, MG Papadopoulos, Computational Studies of Darunavir into HIV-1 Protease and DMPC Bilayer: Necessary Conditions for Effective Binding and the Role of the Flaps, J.Chem. Inf. Model. 52, 1542-1558 (2012).
51) G. Megariotis, A Avramopulos, MG Papadopoulos, H Reis, Computer Simulation of the Linear and Nonlinear Optical Properties of Langmuir-Blodgett Films of a Squaraine derivative, J. Phys. Chem. C 116, 15449-15457 (2012).
52) M. Garcia-Borras, M Sola, D Lauvergnat, H Reis, JM Luis, B Kirtman, A Full Dimensionality Approach to the Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Tunneling Motions, J. Chem. Theo. Comp. 9, 520-532 (2013).
53) Avramopoulos, H Reis, JM Luis, MG Papadopoulos, On the vibrational Linear and Nonlinear Optical Properties of compounds involving noble gas atoms: HXeOXeH, HXeOXeF, and FXeOXeF, J. Comp. Chem. 34, 1446-1455 (2013).
54) Avramopoulos, H. Reis, GA Mousdis, MG Papadopoulos, Ni Dithiolenes – A Theoretical Study on Structure-Propery Relationships, Eur. J. Inorg. Chem. 27, 483-4850 (2013).
55) Coe, A. Avramopoulos, MG Papadopoulos, K Pierloot, S Vancolillie, H. Reis, Theoretical Modeling of Photoswitching of Hyperpolarisabilities in Ruthenium Complexes, Eur. J. Chem. 15, 15955-15963 (2013).
56) H. Reis, J.M. Luis, M. Garcia-Borras, B. Kirtman, Computation of Nonlinear Optical Properties of Molecules with Large Anharmonic Motions. III. Arbitrary Double-Well Potentials, J. Chem. Theo. Comp. 10, 236-242 (2015).
57) H.Reis, B. Rasulev, M.G. Papadopoulos, J. Leszczynski, Reliable but Timesaving: In Search of an Efficient Quantum-chemical Method for the Description of Functional fullerenes, Current Topics in Medicinal Chemistry 2015
58) H. Tzoupis, G. Leonis, A. Avramopoulos, H. Reis, Z. Czyznikowska, S. Zerva, N. Vergadou, L.D. Peristeras, K.D. Papavasileiou, M.N. Alexis, T. Mavromoustakos, M.G. Papadopoulos Elucidation of the binding mechanism of renin using a wide array of computational techniques and biological assays. Journal of molecular graphics & modelling 2015.
59) G.Leonis, A. Avramopoulos, K.D. Papavasileiou, H. Reis, T. Steinbrecher, M.G. Papadopoulos, A Comprehensive Computational Study of the Interaction between Human Serum Albumin and Fullerenes, J. Phys. Chem. B 119, 14971-14985 (2015).
60) D. Lauvergnat, J.M. Luis, B. Kirtman, H. Reis, A. Nauts, Numerical and Exact Kinetic Energy Operator using Eckart Conditions with one or several Reference Conditions, J. Chem. Phys. *Accepted*.

Co-editor

Handbook of Computational Chemistry, *Eds.* J. Leszczynski, A. Kaczmarek-Kedziera, M.G. Papadopoulos, H. Reis, A.J. Sadlej, M.K. Shukla, Springer Reference, 1st Edition 2012; 2nd Edition 2016 (*in progress).*