

MANTHOS G. PAPADOPOULOS**CURRICULUM VITAE**

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I. Nationality

Greek, born in Athens, Greece, in 1948

II. Education

B. Sc in Chemistry, University of Patras, Greece (1971).

Ph. D in Theoretical Chemistry, University of Essex U.K. (1976). The title of the thesis is: "Theoretical studies of NMR chemical shifts, susceptibilities and polarisabilities". The Ph. D work has been completed in three years (1972-1975), the first two of which were spent in Essex under the supervision of Dr R. Jones and the last Cambridge under the guidance of Professor A. D. Buckingham.

III. Military Service

1970-1971.

IV. Scholarships

- (a) The State Scholarship (IKY) awarded for my undergraduate studies.
- (b) A scholarship from Skilitision was received during my Ph. D.

V. Career

- (a) A Postdoctoral fellowship was granted by the Science and Engineering Research Council, University of Bristol (1975-1977).
- (b) Researcher at the National Hellenic Research Foundation since 1979.

VI. Funding

My research has been funded by:

- (a) The British Telecom
- (b) The European Community
- (c) The British Council
- (d) The Royal Society (UK)
- (e) The Engineering and Physical Sciences Research Council (U.K)
- (f) The General Secretariat for Research and Technology
- (g) The European Union:
 - (i) Human Capital and Mobility Network (CHRX-CT93-0334)
 - (ii) TMR Network (FMRX-CT96-0047). In this Network MGP was scientist-in-charge of one of the teams. His node contributed 148 person months of research training to young researchers and 18 joint research papers. Budget: 240.000 euros.
 - (iii) Marie Curie Host Development Fellowship (HPMD-CT-2001-00091). MGP was coordinator. Budget: 114.000 euros.
 - (iv) Marie Curie Host Fellowships (MTKD-CT-2006-042488). Budget: 389.953

euros.

Man-months: 48. Participants: Dr M. G. Papadopoulos, NHRF, Co-ordinator, Professor E. Artacho, University of Cambridge, UK, Dr J. M. Luis, University of Girona, Spain, Professor H. Shinohara, University of Nagoya, Japan, Dr N. Tagmatarchis, NHRF, Greece and Professor B. Kirtman, University of California, Santa Barbara, USA.

- (v) Early Stage Training (MEST-CT 2005-020575). Participation.
Total budget: 984.122 euros.
- (vi) "Advancement of research capability for the development of new functional compounds" [FP7-REGPOT-2009-1]. Participation.
Total Budget: 2.500.000 euros.

VII. Grants in Computing Time for using super-computers

- (a) Two grants by the Science and Engineering Research Council of UK.
- (b) Two grants by MareNostrum (Spain).
- (c) One grant by Terra Grid (USA).

VIII. Post-doctoral Fellows funded by EU

Dr V. Ingamells
 Dr H. Reis
 Dr M. Makowska-Janusik
 Dr A. Grzybowski
 Dr. P. Labeguerie
 Dr. M. Medved
 Dr. O. Loboda
 Dr. R. Zalesny
 Dr. B. Skwara

IX. Graduate Students

S.Raptis (PhD: 2/2000)
 S. Nasiou (PhD: 2/2000)
 A.Avrampoulos (MSc:10/2000; PhD: 5/2004)
 S. Durdagi (PhD: 5/2009)

X. Undergraduate Students

G. Screttas
 M.Theologitis
 M. Moschos

XI. Teaching

After invitation I taught the course of *Computational Chemistry* to post graduate students of "Democritos" and the Chemical Engineering Department of National Technical University. I also taught *Computational Chemistry Techniques* to the postgraduate students of the Early Stage Training Program of our Institute. This is a European Union Program.

XII. Member of Councils

- (a) Member of the Executive Council of the National Hellenic Research Foundation (1994-1995).

- (b) Member of the Advisory Council of the Institute of the Organic and Pharmaceutical Chemistry.

XIII. Other activities

- (a) I have been invited to review articles by many Journals (e.g. Journal of the American Chemical Society, Journal of Chemical Physics, Chemical Physics Letters, Chemical Physics, International Journal of Quantum Chemistry).
- (b) Organizer of special seminars, attended by High School pupils and given by top specialists (usually University Professors).
- (c) Co-organizer of three national conferences in Chemistry.
- (d) Co-organizer of four international Symposia.

XIV. Invitations

I have given lectures to more than 15 Universities and Conferences after invitation.

CLASSIFICATION OF MY PUBLICATIONS

1. *Development and implementation of theoretical procedures*

- a. An approximation for the determination of the dependence of the shielding constant on the electric field [1].
- b. An approach for the calculation of the intermolecular potential energy surfaces [5].
- c. The CHF-PT-EB-CNDO method [6-8, 11,16].
- d. Approximate formula for the determination of γ [20].
- e. Ab initio procedures for the determination of the properties (α , β and γ) [24, 25, 34, 36, 42]. These employ Hartree-Fock and correlated wavefunctions (MP4(SDTQ), CCSD(T) etc).
- f. Implementation of a technique for determination of the basis set superposition error[25,24].
- g. Determination of the many body contributions to the interaction polarizability and second hyperpolarizability [34].
- h. Extension of CHF-PT-EB-CNDO for the study of transition metal containing compounds [26].
- i. An unrestricted Hartree-Fock approach for the determination of α , β and γ [28].
- j. Definition of basis sets for semiempirical computations of α , β and γ [6-9, 15-16, 21-22, 30, 33, 36].
- k. Rules for developing basis sets for the accurate computation of hyperpolarizabilities [49].
- l. Computation of the correlation contribution to the vibrational properties [63].
- m. Methods for the calculation of the macroscopic susceptibilities of crystals[57,58].
- n. Techniques for the macroscopic susceptibilities of liquids [60,66].
- o. A method for the calculation of the vibrational correction to properties at arbitrary reference geometry [68,73].
- p. A procedure for the calculation of the vibrational corrections to static electric properties of diatomics by Numerov-Cooley [70].
- q. Development of a method for the computation of distributed polarizabilities and hyperpolarizabilities [69].

2. *Analysis of chemical problems*

- a. Carbon-13 chemical shifts.
- b. Nuclear screening constants of ^{13}C and ^{19}F [4].
- c. Molecular anions [9,11, 13, 20].
- d. Molecular cations [18, 19].
- e. Study of hydration of N,N-dimethyl acetamide, using theoretical and experimental data [3].
- f. Charge transfer [37,40,41].
- g. Conjugation [37, 40].
- h. Interatomic interactions [25,34].
- i. Intermolecular interactions [17,22, 27, 29, 32, 36, 39].
- j. Intramolecular interactions [11,12,20,23].

- k. Inversion and rotation [12,15].
- l. Isomerism [10, 16, 18, 20, 38]
- m. Stability of dianions [13].
- n. Organometallic compounds [26].
- o. Connection of structure with polarization properties [e.g. 13-15, 18, 31, 33].
- p. Study of trends in:
 - Alkanes [6]
 - Polyenes [7]
 - Aromatics [8,10,15,16]
 - Organolithium compounds [14]
 - Amides [22]
 - Quinones [23]
 - Polythiophenes [40].
- q. Computation of the vibrational effects on the nlo properties [e.g. 50,51,65,70,81].
- r. Design or selection of nlo materials [44,48,79,86,88].
- s. Effect of lithiation on the polarizabilities and hyperpolarizabilities [52,61, 63,72]
- t. Macroscopic nlo properties [57,58,60,66,69,74,77,78].

3. *Study of methodological problems*

- a. Study of correlation effects on the polarizabilities and hyperpolarizabilities [49-52,54,56,59].
- b. Analysis of the basis set effect on the properties (μ , α , β and γ) [49-51,54]
- c. Study of the nlo properties of clusters [67].
- d. Determination of the effect of molecular geometry, using appropriate models with flexible structure, on the polarizabilities and hyperpolarizabilities [59].
- e. Computation of interaction effects on the nlo properties [17,34,55].
- d. Relativistic corrections to polarizabilities and hyperpolarizabilities [64,75,83].
- f. Analysis of the structure-polarization relationship [e.g. 7,13,26,79].

4. *Design of novel nlo materials*

- a. Derivatives involving lithium [52,53,61,63,72].
and transition metals [e.g. 26,45,46,48].

LIST OF PUBLICATIONS

1. Carbon-13 nuclear magnetic resonance studies of piperidine and piperazine compounds. Part II. Empirical substituent parameters for, and the shielding anisotropy of, the N-nitroso-group.
G. E. Ellis, R. G. Jones and M. G. Papadopoulos, *J. Chem Soc., Perkin Transactions II*, 1381, (19974).
2. The anisotropy of the magnetic susceptibility of benzene, 1,3,5-trifluorobenzene and hexafluorobenzene.
B. Day and M. G. Papadopoulos, *Chim. Chronika*, **8**, 131 (1979).
3. Model studies of the first hydration shell of N, N-dimethylacetamide using CNDO/2 viewed in the light of NMR spectroscopic and other experimental evidence.
R. G. Jones and M. G. Papadopoulos, *Chim. Chronika*, **8**, 291 (1979).
4. The polarizability and the nuclear screening constant anisotropies for ^{13}C and ^{19}F in C_6H_6 , 1,3,5- $\text{C}_6\text{H}_3\text{F}_3$ and C_6F_6 .
M. G. Papadopoulos and B. Day, *Chim. Chronika*, **9**, 149 (1980).
5. Direct calculation of intermolecular potential energy surfaces.
J. Gerratt and M. G. Papadopoulos, *Mol. Phys.*, **41**, 1071 (1980).
6. Calculations of induced moments in large molecules. I. Polarizabilities and second hyperpolarizabilities in some alkanes.
C. A. Nicolaides, M. G. Papadopoulos and J. Waite, *Theor. Chim. Acta*, **61**, 427 (1982).
7. Calculations of induced moments in large molecules. II. Polarizabilities and second hyperpolarizabilities of some polyenes.
M. G. Papadopoulos, J. Waite and C. A. Nicolaides, *J. Chem. Phys.*, **77**, 2527 (1982).
8. Calculations of induced moments in large molecules. III. Polarizabilities and second hyperpolarizabilities of some aromatics.
J. Waite, M.G. Papadopoulos and C. A. Nicolaides, *J. Chem. Phys.*, **77**, 2536 (1982).
9. Extended basis CNDO calculations of linear and non linear electric susceptibilities of some molecular dianions and carbanions using coupled Hartree-Fock perturbation theory.
J. Waite and M. G. Papadopoulos, *J. Comp. Chem.*, **4**, 578 (1983).
10. The second hyperpolarizability of 1-nitronaphthalene.
J. Waite and M. G. Papadopoulos, *J. Chem. Phys.*, **80**, 3503 (1984).
11. The variation of calculated electric polarisabilities and hyperpolarisabilities in cycloocta-1,5-diene, annulene, their anions and several of their derivatives, induced by changes in molecular structure and charge: A comparative study.
J. Waite and M. G. Papadopoulos, *J. Mol. Struct.*, **108**, 247 (1984).

12. The variation in the second hyperpolarisability of cyclobutane and cyclopentane through inversion, and an analysis of the contributions to this property.
J. Waite and M. G. Papadopoulos, *Can. J. Chem.*, **62**, 1736 (1984).
13. Electric second hyperpolarizability as a novel probe to the stability of dianions. Case study: four conformers of $C_6H_8^{2-}$.
J. Waite and M. G. Papadopoulos, *J. Org. Chem.*, **49**, 3837 (1984).
14. A study of molecular polarization. The effect of lithiation on the hyperpolarisability of CH_nLi_{6-n} .
J. Waite and M. G. Papadopoulos, *J. Mol. Struct.*, **125**, 155 (1984).
15. The effect of intramolecular processes on the polarizabilities and hyperpolarizabilities of some amines.
J. Waite and M. G. Papadopoulos, *J. Chem. Phys.*, **82**, 1427 (1985).
16. The polarizability and second hyperpolarizability of some azabenzenes.
J. Waite and M. G. Papadopoulos, *J. Chem. Phys.*, **82**, 1435 (1985).
17. The effect of intermolecular interactions on the second hyperpolarisability of the ammonia heptamer.
J. Waite and M. G. Papadopoulos, *Chem. Phys. Letters.*, **114**, 539 (1985).
18. Polarizability and second hyperpolarizability of some molecular cations. The effect of charge variation on these properties.
J. Waite and M. G. Papadopoulos, *J. Phys. Chem.*, **89**, 2291 (1985).
19. The polarizability and second hyperpolarizability of the phenyl cation.
M. G. Papadopoulos and J. Waite, *Z. Naturforsch.*, **40a**, 1140 (1985).
20. The effect of structural changes on the polarisability and second hyperpolarisability in some benzene isomers and their anions.
Waite and M. G. Papadopoulos, *Z. Naturforsch.*, **40a**, 142 (1985).
21. Calculations of induced moments in large molecules. The average polarisability and second hyperpolarisability of some polyacetylenes and a scale of polarization for CH_3 , F, H and NH_2 . A comparative study.
Waite and M. G. Papadopoulos, *J. Chem. Soc., Faraday Trans., II*, **81**, 433 (1985).
22. Calculations of induced moments in large molecules. V. A Study of intermolecular interactions and a functional group analysis of some amides, through the investigation of their polarizabilities and hyperpolarizabilities. A comparative study.
J. Waite and M. G. Papadopoulos, *J. Phys. Chem.*, **83**, 4047 (1985).
23. The polarizability and second hyperpolarizability of some quinones. Analysis of the effect of intra-molecular interactions on the hyperpolarisability.
M. G. Papadopoulos and J. Waite, *J. Phys. Chem.*, **90**, 5491 (1986).

24. The second hyperpolarizability of HCl and the effect of basis set variation on this property in hydrogen fluoride by fully coupled Hartree-Fock perturbation theory with a method for circumventing the transformation of 2-electron integrals. An ab-initio study.
J. Waite and M. G. Papadopoulos, *J. Chem. Phys.*, **85**, 2831 (1986).
25. On the interaction hyperpolarisability of He₂, He₃ and Ne₂. An ab-initio study.
M. G. Papadopoulos and J. Waite, *Chem. Phys. Letters*, **135**, 361 (1987).
26. Calculation of the polarisability and second hyperpolarisability of ferrocene, Fe(C₅H₅)₂, using the extended CHF-PT-EB-CNDO method.
J. Waite and M. G. Papadopoulos, *Z. Naturforsch.*, **42a**, 749 (1987).
27. The effect of intermolecular interactions in some water clusters and hydrates of the hydronium and hydroxyl ions, on their polarisability and hyperpolarisabilities. A comparative study.
J. Waite and M. G. Papadopoulos, *Z. Naturforsch.*, **43a**, 253 (1988).
28. On the study of polarisabilities and hyperpolarisabilities with an unrestricted Hartree-Fock wave function. Case study: HF⁺ and HCl⁺.
J. Waite and M. G. Papadopoulos, *J. Mol. Struct. (Theochem)*, **164**, 413 (1988).
29. The effect of the water-cation interaction on the polarisability and second hyperpolarisability of hydrated Li⁺. A comparative study.
J. Waite and M. G. Papadopoulos, *Can. J. Chem.*, **66**, 1440 (1988).
30. The polarisability and second hyperpolarisability of some biomolecules.
M. G. Papadopoulos and J. Waite, *J. Mol. Struct. (Theochem)*, **170**, 189 (1988).
31. On the hyperpolarisabilities of some alkylbenzenes.
M. G. Papadopoulos and J. Waite, *J. Chem. Soc. Perkin Trans. II*, 2055 (1988).
32. On the electric properties of the benzene dimer.
M. G. Papadopoulos and J. Waite, *J. Mol. Struct. (Theochem)*, **184**, 399 (1989).
33. Calculation of induced moments in large molecules. 6. Scale of polarization for some functional groups. A comparative study.
J. Waite and M. G. Papadopoulos, *J. Phys. Chem.*, **93**, 43 (1989).
34. On the many-body contributions to the interaction polarisability and hyperpolarisability of He_n.
J. Waite and M. G. Papadopoulos, *Theor. Chim. Acta*, **75**, 53 (1989).
35. Relationships of the polarisability with the number of valence electrons, the total energy and the second hyperpolarisability of methylbenzenes.
J. Waite and M. G. Papadopoulos, *J. Naturforsch.*, **44a**, 591 (1989).
36. Variation of the second hyperpolarisability of (HF)_n induced by changes in structure. A comparative study.

- M. G. Papadopoulos and J. Waite, *J. Chem. Soc., Faraday Trans. II*, **85**, 1885 (1989).
37. On the effect of the conjugation and charge transfer on the polarisability, first and second hyperpolarisabilities of some polyenes and nitro-polyenes.
M. G. Papadopoulos and J. Waite, *J. Mol. Struct. (Theochem.)*, **202**, 121 (1989).
38. The dependence of the polarizability, α , and the hyperpolarizabilities β and γ in a series of nitrogen heterocyclics, on their molecular structure. A comparative study.
J. Waite and M. G. Papadopoulos, *J. Phys. Chem.*, **94**, 1755 (1990).
39. The effect of H-bond interactions on the first hyperpolarisability of $(HF)_n$. A comparative study.
J. Waite and M. G. Papadopoulos, *Z. Naturforsch.*, **45a**, 189 (1990).
40. The effect of the charge transfer on the polarizability and hyperpolarizabilities of some selected, substituted polythiophenes. A comparative study.
J. Waite and M. G. Papadopoulos, *J. Phys. Chem.*, **94**, 6244 (1990).
41. Analysis of some significant process for molecular polarization.
M. G. Papadopoulos and J. Waite, *J. Chem. Soc., Faraday Trans.*, **86**, 3525 (1990).
42. The effect of the basis set variation and correlation on the second hyperpolarizability of H_2O .
M. G. Papadopoulos and J. Waite, *J. Mol. Struct. (Theochem)*, **235** 137 (1991).
43. Theoretical study of 1-benzoyloxy-4,5-dimethyl-1,2,3-triazole and its corresponding N-acyl isomers using the AM1 method.
A. B. Theocharis, N E. Alexandrou, M. G. Papadopoulos and J. Waite, *J. Chem. Res. (S)*, 104 (1991).
44. Polarization mechanisms and properties of some substituted ferrocenes. A comparative study.
J. Waite and M. G. Papadopoulos, *J. Phys. Chem.*, **95**, 5426 (1991).
45. Interpretation of the second hyperpolarizability of $Ni(S_2C_2H_2)_2$ and some of its derivatives. A comparative study.
M. G. Papadopoulos and J. Waite, C. S. Winter and S. N. Oliver, *Inorg. Chem.*, **32**, 277 (1993).
46. On the design of molecules with large nonlinearities.
J. Waite and M. G. Papadopoulos, *Nonlinear Optics*, **6**, 297 (1994).
47. Analysis of the polarizability and second hyperpolarizability of α,ω dithienylpolyenes.
M. G. Papadopoulos and J. Waite, *Nonlinear Optics*, **7**, 65 (1994).
48. Some dithiolene derivatives of Pd with large second hyperpolarizability.
M. G. Papadopoulos and J. Waite, *Optical Materials*, **3**, 145 (1994).

49. Rules for developing basis sets for the accurate computation of hyperpolarizabilities. Application to He, H₂, Be, Ne, F⁻ and HF.
M. G. Papadopoulos and J. Waite and A. D. Buckingham, *J. Chem. Phys.*, **102**, 371 (1995).
50. The static electronic and vibrational polarizabilities and hyperpolarizabilities of Li₂.
M. G. Papadopoulos, A. Willetts and N. C. Handy, *Mol. Phys.*, **85**, 1193 (1995).
51. The static polarizabilities and hyperpolarizabilities of LiH: Electronic and vibrational contributions.
M. G. Papadopoulos, A. Willetts and N. C. Handy, *Mol. Phys.*, **88**, 1063 (1996).
52. Organolithium and organosodium compounds. The second hyperpolarizabilities of C₈H₈Li₂ and C₈H₈Na₂.
M. G. Papadopoulos, S. G. Raptis and I. N. Demetropoulos, *Mol. Phys.*, **92**, 547 (1997).
53. Some organic and organometallic molecules with remarkably large second hyperpolarizabilities.
M. G. Papadopoulos, S. G. Raptis, I. N. Demetropoulos and S. M. Nasiou, *Theor. Chem. Acc.*, **99**, 124 (1998).
54. The electronic, vibrational and rotational contributions to the dipole moment, polarizability, and first and second hyperpolarizabilities of the BH molecule.
V. E. Ingamells, M. G. Papadopoulos, N. C. Handy and A. Willetts, *J. Chem. Phys.*, **109**, 1845 (1998).
55. Interaction effects on electric susceptibilities: A model study of polarizabilities of the Be atom embedded in He clusters.
M. G. Papadopoulos and A. J. Sadlej, *Chem. Phys. Letters*, **288**, 377 (1988)
56. On the ground state of NiH₂.
M. Barysz and M. G. Papadopoulos, *J. Chem. Phys.*, **109**, 3699 (1998).
57. Calculation of macroscopic first, second and third-order optical susceptibilities of the urea crystal.
H. Reis, M. G. Papadopoulos and R. W. Munn, *J. Chem. Phys.*, **109**, 6828 (1998).
58. Calculation of macroscopic first and third-order optical susceptibilities for the benzene crystal.
H. Reis, S. Raptis, M. G. Papadopoulos, R. H. C. Janssen, D. N. Theodorou and R. W. Munn, *Theor. Chem. Acc.*, **99**, 384 (1998).
59. The static and frequency dependent polarizabilities and hyperpolarizabilities of H₂S_n.
S. G. Raptis, S. M. Nasiou, I. N. Demetropoulos and M. G. Papadopoulos, *J. Comp. Chem.*, **19**, 1698 (1998).

60. Computer simulation of the linear and nonlinear optical properties of liquid benzene: Its local fields, refractive index and nonlinear susceptibility.
R. H. C. Janssen, J. M. Bomont, D. N. Theodorou, S. Raptis and M. G. Papadopoulos, *J. Chem. Phys.*, **110**, 6463 (1999).
61. The polarizability and the second hyperpolarizability of the tetrakis (phenylethenyl) ethene and several of its derivatives.
M. Theologitis, G. C. Screttas, S. G. Raptis and M. G. Papadopoulos, *Int. J. Quant. Chem.*, **72**, 177 (1999).
62. Nonlinear optical properties of a B₄ cluster.
H. Reis and M. G. Papadopoulos, *J. Comp. Chem.*, **20**, 679 (1999).
63. Συνδυασμός χρήσης πυρηνικού μαγνητικού συντονισμού και υπολογιστικής χημείας στο σχεδιασμό πεπτιδομιμητικών ανταγωνιστών του υποδοχέα της αγγειοτασίνης II, μιας νέας υποσχόμενης γενεάς αντιυπερτασικών φαρμάκων.
Α. Κολοκούρης, Θ. Μαυρομούστακος, Μ. Ζερβού, Ρουμελιώτη, Ι. Ματσούκας, Μ. Παπαδόπουλος, και Σ. Ράπτης, *Φαρμακευτική*, **11**, 125 (1999).
64. Vibrational effects on the polarizability and second hyperpolarizability of ethylene.
V. E. Ingamells, M. G. Papadopoulos and S. G. Raptis, *Chem. Phys. Letters*, **307**, 484 (1999).
65. The correlation, relativistic, and vibrational contributions to the dipole moments, polarizabilities, and first and second hyperpolarizabilities of ZnS, CdS, and HgS. S. G. Raptis, M. G. Papadopoulos and A. J. Sadlej, *J. Chem. Phys.*, **111**, 7904 (1999).
66. Molecular simulation of static hyper-Rayleigh scattering: A calculation of the dipolarization ratio and the local fields for liquid nitrobenzene.
R. H. C. Janssen and D. N. Theodorou, S. Raptis and M. G. Papadopoulos, *J. Chem. Phys.*, **111**, 9711 (1999).
67. DFT calculations of static dipole polarizabilities and hyperpolarizabilities for the boronclusters B_n, (n=3-8,10).
H. Reis, M. G. Papadopoulos and I. Bustani, *Int. J. Quant. Chem.*, **78**, 131 (2000).
68. Vibrational corrections to properties at arbitrary reference geometry.
V. E. Ingamells, M. G. Papadopoulos and A. J. Sadlej, *J. Chem. Phys.*, **112**, 1645 (2000).
69. Distributed first and second hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals.
H. Reis, M. G. Papadopoulos, C. Hättig, J. G. Angyan and R. W. Munn, *J. Chem. Phys.*, **112**, 6161 (2000).
70. Vibrational corrections to static electric properties of diatomics by Numerov-Cooley integration.
V. E. Ingamells, M. G. Papadopoulos and A. J. Sadlej, *Chem. Phys. Letters*, **316**, 541 (2000).

71. Polarizabilities of azabenzenes.
P. Calaminici, K. Jug, A. M. Koster, V. E. Ingamells and M. G. Papadopoulos, *J. Chem. Phys.*, **112**, 6301 (2000).
72. Hexalithiobenzene: A molecule with exceptionally high second hyperpolarizability.
S. G. Raptis, M. G. Papadopoulos and A. J. Sadlej, *Phys. Chem. Chem. Phys.*, **2**, 3393 (2000).
73. Vibrational corrections to linear and nonlinear electric properties of polyatomic molecules at arbitrary reference geometry.
V. E. Ingamells, M. G. Papadopoulos and A. J. Sadlej, *Chem. Phys.*, **260**, 1 (2000).
74. Calculation of macroscopic linear and nonlinear optical susceptibilities for the naphthalene, anthracene and meta-nitroaniline crystals.
H. Reis, M. G. Papadopoulos, P. Calaminici, K. Jug and A. M. Köster, *Chem. Phys.*, **261**, 359 (2000).
75. Vibrational corrections to electric properties of relativistic molecules: The coinage metal hydrides.
A. Avramopoulos, V. E. Ingamells, M. G. Papadopoulos and A. J. Sadlej, *J. Chem. Phys.*, **114**, 198 (2001).
76. Vibrational effects on electric properties of cyclopropanone and cyclopropanethione.
U. Eckart, V. E. Ingamells, M. G. Papadopoulos and A. J. Sadlej, *J. Chem. Phys.*, **114**, 735 (2001).
77. Calculation of refractive indices and third-harmonic generation susceptibilities of liquid benzene and water: Comparison of continuum and discrete local-field theories.
H. Reis, M. G. Papadopoulos and D. N. Theodorou, *J. Chem. Phys.*, **114**, 876 (2001).
78. Electrostatic calculation of linear and non-linear optical properties of iceI_H, II, IX and VIII.
H. Reis, S. G. Raptis and M. G. Papadopoulos, *Chem. Phys.*, **263**, 301 (2001).
79. Comparison of the non-linear optical properties of a dimethylaminostilbene derivative containing a molybdenum mononitrosyl redox center and of p,p'-dimethylaminonitrostilbene, calculated by ab-initio methods.
H. Reis, S. G. Raptis and M. G. Papadopoulos, *Phys. Chem. Chem. Phys.*, **3**, 3901 (2001).
80. Synthesis of N-urethane-protected γ -amino-functionalized butenoates and tautomeric studies by means of NMR, X-ray crystallography and ab initio calculations.
A. Detsi, E. Gavrielatos, M.-A. Edam, O. Igglessi-Markopoulou, J. Markopoulos, M. Theologitis, H. Reis and M. Papadopoulos, *Eur. J. Org. Chem.*, 4337 (2001).
81. Trends in the electronic and vibrational contributions to the dipole moment, polarizabilities, first and second hyperpolarizabilities of the hydrides of Li, Na and K.
A. Avramopoulos and M. G. Papadopoulos, *Mol. Phys.*, **100**, 821 (2002).

82. Local electric fields and distributed response: Electric susceptibility calculations for molecular materials.
R. W. Munn, M. G. Papadopoulos and H. Reis, *Polish, J. Chem.*, **76**, 155 (2002).
Invited article.
83. Relativistic effects on interaction-induced electric properties of weakly interacting systems: The HF...AuH dimer.
A. Avramopoulos, M. G. Papadopoulos and A. J. Sadlej, *J. Chem. Phys.*, **117**, 10026 (2002).
84. Strong interactions through the X...Au-X bridge: the Au bond?
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BOOKS

Edited by M. G. Papadopoulos

1. Title: “*Nonlinear optical responses of molecules, solids and liquids: Methods and applications*”, Research Sighnpost, Trivandrum (2003).
2. Title: “*Nonlinear optical properties of matter: From molecules to condensed phases*”.
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3. I am co-editor of two books which will be published in 2010:
 - (i) “Linear scaling techniques in computational chemistry and physics: Methods and Applications”. Co-editors: J. Leszczynski, P. Mezey and R. Zalesny, Publisher: Springer.

(ii) “Solids and nanostructures”. Co-editor: H. Reis. Publisher: World Scientific.

INTERNATIONAL SYMPOSIA

I have co-organized 4 International Symposia.