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- Nationality* Greek, born in Athens, Greece, in 1948
- 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.
- Military Service* 1970-1971.
- Scholarships* (a) The State Scholarship (IKY) awarded for my undergraduate studies.
(b) A scholarship from Sklitsion was received during my Ph. D.
- 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.
- Research interests* Most of my work deals with the study of the molecular polarizability (α) and the hyperpolarizabilities (β and γ) of organic molecules. Through them, it is expected to illuminate various aspects of the molecular structure. The derived know-how is used for the design of nonlinear optical materials for industrial applications. The properties of interest are computed by employing semiempirical and ab initio techniques.
- 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.) participate in a Human Capital and Mobility Network and in a TMR (Training and Mobility of Researchers) Research Network. These networks aim at designing and synthesizing novel NLO materials. In the first Network I am co-organizer of the theory group and in the second assistant coordinator and Physical Sciences Research Council of Britain. The first two were in cooperation with Professor A. D. Buckingham (University of Cambridge) and the third was cooperation with Professor A. E. Underhill (University of Wales).
- Other activities* (a) I have been invited to review articles by the:
(i) Journal of the American Chemical Society
(ii) International Journal of Quantum Chemistry
(iii) Chemical Physics Letters
(b) Member of the Executive Council of the National Hellenic Research Foundation (1994-1995)

- (c) Organizer of special seminars, attended by High School pupils and given by top specialists (usually University Professors).
- (d) Co-organizer of three national conferences in Chemistry.

CLASSIFICATION OF MY PUBLICATIONS

1. Development 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)].
- 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 for the accurate computation of hyperpolarizabilities [49].
- l. Computation of the correlation contribution to the vibrational properties [63]

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 vibrational effects [50].
- r. Design or selection of nlo materials [44-48].
- s. Effect of lithiation on the polarizabilities and hyperpolarizabilities [52,61, 63]

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. Computation of the vibrational and rotational contributions to the nlo properties [50,51,54].
- d. Determination of the effect of molecular geometry, using appropriate models with flexible structure, on the polarizabilities and hyperpolarizabilities [59].
- e. Calculation of first, second and third order optical susceptibilities of crystals [57,58].
- f. Computer simulation of linear and nonlinear optical properties of liquids [57].
- g. Computation of the interaction effects on the hyperpolarizabilities [55].
- h. Computation of the rotational and vibrational contribution to nlo prperties [50,51,54,64].
- i. Computation of interaction effects on the electric hyperpolarizabilities [17,34,55].
- j. Relativistic corrections to polarizabilities and hyperpolarizabilities[64,83,84,85]
- k. Condensed phases [69,74,78,89,92].

4. Design of novel NLO materials

- a. Derivatives involving lithium [52,53,61,63].
and transition metals [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).

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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.
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J. Waite and M. G. Papadopoulos, *Can. J. Chem.*, **62**, 1736 (1984).
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15. The effect of intramolecular processes on the polarizabilities and hyperpolarizabilities of some amines.
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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.
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20. The effect of structural changes on the polarisability and second hyperpolarisability in some benzene isomers and their anions.
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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.
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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.
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34. On the many-body contributions to the interaction polarisability and hyperpolarisability of He_n.
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S. G. Raptis, S. M. Nasios, I. N. Demetropoulos and M. G. Papadopoulos, *J. Comp. Chem.*, **19**, 1698 (1998).
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BOOKS

1. Edited by M. G. Papadopoulos.
Title: Nonlinear optical responses of molecules, solids and liquids: Methods and applications. Research Signpost, Trivandrum, India (2003).
2. Provisional title: "Nonlinear optical properties of matter: From molecules to condensed phases".
Editors: M. G. Papadopoulos, J. Leszczynski and A. J. Sadlej. It will be published by Springer later this year. It involves 21 articles written by some of the top experts (experimentalists and theoreticians). The introduction has been written by Professor M. A. Ratner.

CONFERENCES

I have participated in several national and international conferences. Some of the more recent participations involve:

1. Μη γραμμικές οπτικές ιδιότητες εύκαμπτων μοριακών αλυσσίδων.
Σ. Νάσιου, Γ. Ν. Δημητρόπουλος, Μ. Γ. Παπαδόπουλος και Σ. Ράπτης,
16^ο Πανελλήνιο Συνέδριο Χημείας (1995).
2. The static polarizabilities and hyperpolarizabilities of LiH: Electronic and vibrational contributions.
M. G. Papadopoulos, A. Willetts, N. C. Handy and A. E. Underhill, International Conference: "*Molecular Quantum Mechanics: Methods and Applications*", Cambridge (1995).
3. The vibrational contributions to polarizabilities and hyperpolarizabilities.
V. E. Ingamells and M. G. Papadopoulos, International Conference: "*Optical Electric and Magnetic Properties of Molecules*", Cambridge (1997).
4. Lithium substitution as a factor for the enhancement of the non-linear optical properties of conjugated organic compounds.
M. G. Papadopoulos, G. C. Screttas, S. G. Raptis, and M. E. Theologitis, "*Organic and Photonic Materials and Devices*", SPIE Photonics West '99, 23-29 January 1999, San Jose CA, USA.
5. The polarizabilities and hyperpolarizabilities of lithiated derivatives. M. G. Papadopoulos, S. G. Raptis and V. E. Ingamells, "*5th World Congress of Theoretically Oriented Organic Chemists, WATOC '99*", London 1999.
6. The relativistic, correlation and vibrational contributions to non-linear optical properties of ZnS, CdS and HgS, S. G. Raptis and A. J. Sadlej, "*5th World Congress of Theoretically Oriented Organic Chemists, WATOC '99*", London 1999.
7. Computational methods for the prediction of vibrational contributions to non-linear optical properties.
V. E. Ingamells and M. G. Papadopoulos, "*5th World Congress of Theoretically Oriented Organic Chemists, WATOC '99*", London 1999.
8. Macroscopic optical first to third order susceptibilities of molecular crystals, calculated from molecular ab-initio (hyper)polarizabilities.
H. Reis, M. G. Papadopoulos and R. W. Munn, "*5th World Congress of Theoretically Oriented Organic Chemists, WATOC '99*", London 1999.
9. Molecular structure of magnesium-urea complexes.
S. Raptis, J. Anastosopoulou, M. Papadopoulos and T. Theophanides, "*XXVIIeme Colloque Francais sur le magnesium 27 Novembre 1999*", "*Pharmacological properties and indications of magnesium*", Chatenay-Malabry, 1999.
10. Computation of the non-linear optical properties of molecules, liquids and solids.
M. G. Papadopoulos, H. Reis, D. N. Theodorou and S. G. Raptis, in "*Atoms, Molecules and Quantum Dots in laser Fields: Fundamental Processes*", edited by N. Bloembergen, N. Rahman and A. Rizzo, Pisa, 12-16 June 2000.
11. Δονητικές και σχετικιστικές διορθώσεις στη διπολική ροπή, πολωσιμότητα και την πρώτη υπερπολωσιμότητα των υδριδίων του Cu, Ag και Au.
Α. Αβραμόπουλος, V. E. Ingamells, Μ. Γ. Παπαδόπουλος και Α. J. Sadlej,
18ο Πανελλήνιο Συνέδριο Χημείας, 10-13 Μαρτίου 2001, Εκθεσιακό Κέντρο Οργανισμού Λιμένα Πειραιά.

12. Conformation dependence of the excitation spectrum and electro-optical properties of 3-aminoacroleine.
M. Jablonski, A. Avramopoulos, M. G. Papadopoulos and A. J. Sadlej, First European Symposium on Theoretical Chemistry, 28-30 October 2002, Zwettl, Austria.
13. Σύνθεση νέων νευροστεροειδών αγωνιστών στους GABAA υποδοχείς.
N. Αυλωνίτης, Χ. Σούλη, Ε. Λέκκα, Θ. Καλογεροπούλου, Α. Τσοτίνης, Α. Μακρυγιάννης, Η. Reis και Μ. Γ. Παπαδόπουλος, 19^ο Πανελλήνιο Συνέδριο Χημείας, Πανεπιστήμιο Κρήτης, 6-10 Νοεμβρίου 2002.
14. The polarizabilities and hyperpolarizabilities of HArF, M. G. Papadopoulos, A. Avramopoulos and H. Reis, Molecular Quantum Mechanics: The No Nonsense Path to Progress, An International Conference in Honour of Nicholas Handy, July 24-29, 2004, St John's College, Cambridge University, England.
15. On the vibrational polarizabilities and hyperpolarizabilities. Analysis of some specific examples: Pyrrole and HArF.
M. G. Papadopoulos, A. Avramopoulos and H. Reis, ICCMSE 2004, 19-23 November 2004, Athens. Invited Speaker.
16. A comparative study of the polarizability and hyperpolarizabilities of some Zn clusters.
M. G. Papadopoulos, H. Reis, A. Avramopoulos, S. Erkoc and L. Amirouche.
COST Meeting in Edinburgh, 5-8/5, 2005.

MINI-SYMPOSIUM

MGP and Professor B. Kirtman currently organize a mini-symposium on the vibrational contributions to the linear and non-linear optical properties. This will be part of the International Conference of Computational Methods in Sciences and Engineering 2005 (ICCMSE 2005), which will take place at the Hotel Poseidon Resort, Loutraki, Korinthos, Greece, 21-26 October 2005. Eleven researchers have already accepted to present contributions in this mini-symposium.