George Maroulis

Greek, born 1953.

Professor of Chemistry
University of Patras.

Research interests :
Computational Quantum Chemistry, Chemical Physics, Mathematical Chemistry.

Curriculum Vitae

Patras, 30 June 2014

George Maroulis

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Personal Data Date of birth: June 15, 1953.
Place of birth: Nikea(Piraeus), Greece.
Nationality: Hellenic.
Military service: April 9, 1981, to April 9, 1982.
Married to Anastasia Antonopoulou.
Father of four children, Penthesileia, Neoptolemos, Ianthe and Diomedes.

Education Ptychion (1976, Chemistry), National and Capodistriac University of Athens.
D.Sc. (1981, Quantum Chemistry), Université Catholique de Louvain.
Thèse annexe:
The Many-Universes Interpretation of Quantum Mechanics.
Thèse:
Molecular properties and basis set quality. An approach based on Information Theory.
Awarded the **Prix Pierre Bruylants (1886-1950)** for this Dissertation in 1982.

Positions February-April 1983
Researcher, Laboratoire de Chimie Quantique, Université Catholique de Louvain

August 1983-August 1984
Post-doctoral Fellow, Chemistry Department, University of Ottawa.

January-February 1985
Researcher, Laboratoire de Chimie Quantique, Université Catholique de Louvain

January-August 1986
Researcher, Laboratoire de Chimie Quantique, Université Catholique de Louvain

February 1987-September 1988
Post-doctoral Fellow, Department of Chemistry, University of New Brunswick.

February 1989-May 1993
Assistant Professor, Department of Chemistry, University of Patras.

May 1993 – June 1998
Associate Professor, Department of Chemistry, University of Patras.

June 1998 – Present
Professor, Department of Chemistry, University of Patras.

1991-2000

Visiting Professor, Department of Mathematics, University of the Aegean.

Also,

July-August 1989
Visiting Scientist, Department of Chemistry, University of New Brunswick.

July-August 1990
Visiting Scientist, Department of Chemistry, University of New Brunswick.

March-May 1994
Visiting Professor, Laboratoire de Chimie Structurale, Université de Pau et des Pays de l'Adour, France.

May 1996
Visiting Professor, Laboratoire de Chimie Structurale, Université de Pau et des Pays de l'Adour, France.

September-December 2001
Visiting Professor, Laboratoire de Chimie Structurale, Université de Pau et des Pays de l'Adour, France.

September 2002
Visiting Professor, Laboratoire de Chimie Structurale, Université de Pau et des Pays de l'Adour, France.

September 2004
Visiting Professor, Laboratoire de Chimie Structurale, Université de Pau et des Pays de l'Adour, France.

May-June 2008
Visiting Professor, Groupe de Chimie Théorique et Réactivité, ECP, IPREM UMR 5254, Université de Pau et des Pays de l'Adour, France.

May-June 2011
Visiting Professor, Groupe de Chimie Théorique et Réactivité, ECP, IPREM UMR 5254, Université de Pau et des Pays de l'Adour, France.

Academic

1995-1997
Vice Chairman of the Department of Chemistry, University of Patras.
1997-1999
Chairman of the Department of Chemistry, University of Patras.

Awards

1982: Awarded the **Prix Pierre Bruylants (1886-1950)**.
2004: Prize of the **European Society of Computational Methods in Sciences and Engineering (ESCMSE)** for outstanding work on Computational and Theoretical Chemistry.

Research Interests

1. **Ab Initio** quantum chemical calculations of atoms, molecules, clusters and solids.
2. Modelling the properties of molecules of pharmacological interest.
3. Graph theoretic aproach to pattern recognition, clustering and clsassification in spaces of theoretical descriptions of molecular systems. Analysis of the performance of quantum chemical methods over arbitrary classes of atomic and molecular properties.

Specific thematic classification of areas of research activity

A. **Materials Science.** Nonlinear Optical properties (NLO). Design of materials with specific or enhanced NLO.
B. **Environmental Sciences**. Fundamental Physicochemical properties and intermolecular interactions of water, ozone, nitrogen, carbon dioxide, sulphur dioxide and carbon monoxide. Spectroscopical detection.
C. **Computational Medicinal Chemistry**. Molecular Descriptors of molecules of pharmacological interest and analysis of pharmacological activity.

Research Projects/Networks

2000-2003
Caratheodory Grant, University of Patras (Grant N^o 02449)
Project title: *Systematic study of the nonlinear optical properties of substituted diacetylenes. Correlation of electronic structure and molecular properties.*
2003-2006
European Thematic network (COST ACTION N^o 26, Working group N^o D26/0013/02)
Development of Density Functional Theory models for an accurate description of electronic properties of materials possessing potential high non-linear optical properties

Referee for the following Scientific Journals

1. The Journal of Chemical Physics
2. Journal of the American Chemical Society
3. Journal of Physical Chemistry A
4. Journal of Physical Chemistry B
5. Journal of Physical Chemistry C
6. Journal of Physical Chemistry Letters
7. Physical Review Letters
8. Physical Review B
9. Journal of Chemical Theory and Computation (JCTC)
10. Biochemistry
11. Chemical Physics Letters
12. Chemical Physics
13. Molecular Physics
14. Physical Chemistry Chemical Physics
15. Journal of Physics B Atomic, Molecular and Optical Physics
16. Journal of Physics D Applied Physics
17. Journal of Physical Organic Chemistry
18. International Journal of Quantum Chemistry
19. Journal of Computational Chemistry

20. Computational and Theoretical Chemistry
21. Physica Status Solidi
22. ChemPhysChem
23. Journal of Computational and Theoretical Nanoscience (JCTN)
24. Molecules
25. ACH_Models in Chemistry
26. Zeitschrift fuer Physikalische Chemie
27. New Journal of Physics
28. Synthetic Metals
29. Journal of Molecular Modelling
30. Inorganic Chemistry
31. Journal of Polymer Science Part B: Polymer Physics
32. Physica Scripta
33. Chemistry, A European Journal
34. Crystal Growth and Design
35. Physica B
36. Physica E
37. Journal of Physics and Chemistry of Solids
38. Theoretical Chemistry Accounts
39. Collection of Czechoslovak Chemical Communications
40. Journal of Material Chemistry
41. Spectrochimica Acta A
42. Acta Biomaterialia
43. European Polymer Journal
44. Journal of Theoretical and Computational Chemistry (JTCC)
45. European Journal of Medicinal Chemistry
46. Journal of Physics: Condensed Matter
47. Indian Journal of Physics
48. Journal of Advanced Research
49. Zeitschrift für Naturforschung A
50. Structural Chemistry
51. Organic and Biomolecular Chemistry
52. Journal of Solid State Chemistry
53. European Physical Journal D
54. Physical Chemistry Research
55. Journal of Organic Chemistry
56. Nanoscale
57. ChemPlusChem
58. Chemical Society Reviews
59. Journal of Molecular Structure
60. Medicinal Chemistry Research

Editor of Scientific Journals

Editor-in-Chief
Journal of Computational Methods in Science and Engineering (IOS Press)
Section C: Computational Biology and Medicine
Section D: Computational Chemistry and Physics

Editor-in-Chief
Computing Letters (VSP Brill)
Section C: Computational Biology and Medicine
Section D: Computational Chemistry and Physics

Editor and Founder
Book Series: **SpringerBriefs in Electric and Magnetic Properties of Atoms, Molecules, and Clusters, Springer**, Berlin

Member of Editorial Boards

Member of the Editorial Board
Computational and Theoretical Chemistry (Elsevier)
[*from* ***January 1, 2011***]

Honorary Editorial Board
Reports in Theoretical Chemistry (Dove Press)
[*from* ***August 2011***]

SpringerBriefs in Electric and Magnetic Properties of Atoms, Molecules, and Clusters,
Springer, Berlin

Editor and Founder: Professor George Maroulis
University of Patras, Department of Chemistry, Patras, Greece

SpringerBriefs in Electrical and Magnetic Properties of Atoms, Molecules, and Clusters presents concise summaries of cutting-edge research and practical applications across a wide spectrum of fields centered around linear and non-linear optics, non-linear optical materials, molecular magnets and magnetic materials, and simulations of fluids.

Volumes Published

1. **Sven Heiles and Rolf Schäfer**, Dielectric properties of isolated clusters.
2. **Roberto Cammi**, Molecular response functions for the polarizable continuum model.
3. **Masayoshi Nakano**, Excitation energies and properties of open-shell singlet molecules.
4. **Vladimir Goncharov**, Non-linear optical response in Atoms, Molecules and Clusters.
5. **Stavros C.Farantos**, Non-linear Hamiltonian mechanics applied to molecular dynamics.

6. Organization of Conferences

1. Member of the Scientific Committee: **International Conference of Computational Methods in Sciences and Engineering 2003** (ICCMSE 2003, Kastoria Greece, 12-16 September 2003).
2. Member of the Scientific Committee: **International Conference of Computational Methods in Sciences and Engineering 2004** (ICCMSE 2004, Attica, Greece, 19-24 November 2004).
3. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2005** (ICCMSE 2005, Loutraki, Greece, 21-26 October 2005).
4. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2006** (ICCMSE 2006, Chania, Greece, 27 October – 1 November 2006).
5. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2007** (ICCMSE 2007, Corfu, Greece, 25 – 30 September 2007).
6. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2008** (ICCMSE 2009, Hersonissos, Crete, Greece , 25 - 30 September 2008).
7. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2009** (ICCMSE 2009, Rhodes, Greece, 29 September – 4 October 2009).
8. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2010** (ICCMSE 2010, Kos, Greece, 3 – 8 October 2010).
9. Co-Chairman: **International Conference of Computational Methods in Sciences and Engineering 2011** (ICCMSE 2011, Halkidiki, Greece, 2 – 7 October 2011).

Organization of Symposia in International Conferences

1. ***Computational Methods for the Molecular Sciences*** (ICCMSE 2003, Kastoria Greece, 12-16 September 2003).
2. ***Computational Molecular Science: From atoms and molecules to clusters and materials*** (ICCMSE 2004, Vouliagmeni, Athens, Greece, 19-24 November 2004).
3. ***Electric (hyper)polarizability: From atoms and molecules to the nonlinear optics of materials*** (ICCMSE 2005, Loutraki, Corinth, Greece, 21-26 October 2005).
4. ***Trends and perspectives in Computational Chemistry*** (ICCMSE 2005, Loutraki, Corinth, Greece, 21-26 October 2005).
10. ***Computational Quantum Chemistry: Applications from the atomic to the nanoscale.*** (ICCMSE 2006, Chania, Greece, 27 October – 1 November 2006).
11. ***Computational Spectroscopy*** (with B.Champagne, U.Hohm and C.Pouchan). (ICCMSE 2006, Chania, Greece, 27 October – 1 November 2006).
12. ***The Rodney Bartlett Honour Symposium*** (with A.J.Thakkar and H.Murakami). (ICCMSE 2007, Corfu, Greece, 25 September – 30 September 2007).
13. ***Computational Quantum Chemistry: from atoms and molecules to clusters and nano-objects*** (with D.Xenides and P.Karamanis) (ICCMSE 2008, Heraklion, Greece, 25-30 September 2008).
14. ***Computational Quantum Chemistry*** (**The Symposium is dedicated to the memory of David M.Bishop (1936-2008)).** (ICCMSE 2009, Rhodes, Greece, 29 September 4 October 2009).
15. ***Computational Quantum Chemistry Symposium*** **(**ICCMSE 2010, Kos, Greece, 3-8 October 2010).
16. ***From Small Clusters to Functional Building Blocks of Novel Nanomaterials*** (with C.Pouchan, D.Xenides and P.Karamanis) **(**ICCMSE 2010, Kos, Greece, 3-8 October 2010).
17. ***Computational Quantum Chemistry (Dedicated to Professor Claude Pouchan's contribution to European Science)*** (ICCMSE 2011, Halkidiki, Greece, 2-7 October 2011).

Supervised Doctoral Dissertations

1. Demetrios Xenides
   *A theoretical study of the electric multipole moments, dipole polarizability and hyperpolarizability of the open and ring structure of O_3, S_3, Se_3, Te_3 and SO_2, SeO_2, TeO_2 based on **ab initio** and DFT quantum chemical methods*
   Department of Chemistry, University of Patras (2001).
2. Panaghiotis Karamanis
   Contribution to the systematic study of substitution effects on the linear and nonlinear polarizability of hydrocarbons with conjugated bonds
   Department of Chemistry, University of Patras (2004).
3. Anastasios Haskopoulos
   ***Ab initio** quantum chemical study of the intermolecular interactions of molecules of particular importance to Environmental Sciences.*
   Department of Chemistry, University of Patras (2005)
4. Emmanuel Menadakis
   Quantum chemical study of calcium carbonate
   Department of Chemistry, University of Patras (2005).
5. Agesilaos Chantzis
   Electric multipole moments of subsitituted acetylenic chains $H\text{-}(C{\equiv}C)_n\text{-}H$, $X\text{-}(C{\equiv}C)_n\text{-}H$ and $X\text{-}(C{\equiv}C)_n\text{-}X$, electric (hyper)polarizability of acetylenic chains $H\text{-}(C{\equiv}C)_n\text{-}H$ and interaction induced electric properties for $H\text{-}(C{\equiv}C)_n\text{-}H\cdots He$.
   Department of Chemistry, University of Patras (2011).
6. Constantinos Makris
   Systematic construction of basis sets for the quantum chemical calculation of molecular electric properties. Application to dihalogens XY (X,Y = F, Cl, Br and I)].
   Department of Chemistry, University of Patras (2012).

Published work

Approximately **190** original papers (including four chapters in books) in various international Journals (Journal of Chemical Physics, Journal of Physical Chemistry A and B, Physical Review A, Chemical Physics Letters, Chemical Physics, Theoretical Chemistry Accounts, Molecular Physics, Journal of Physics B: Atomic, Molecular and Optical Physics, International Journal of Quantum Chemistry, etc.). Editor of 15 books. More than **4300** citations in Scientific Journals and related publications. **Hirsch-index 42**.

Books

1. Theodore Simos and George Maroulis, Editors.
   International Conference of Computational Methods in Sciences And Engineering
   Lecture Series on Computer and Computational Sciences, Vol 1.
   VSP Brill, Leiden (2004) (ISBN 90-6764-418-8).

2. George Maroulis, Editor.
   Computational aspects of electric polarizability calculations: Atoms, molecules and clusters.
   IOS Press, Amsterdam (2004) (ISBN 1 58603 495 2)
   Second Edition
   IOS Press, Amsterdam (2006) (ISBN 1-58603-643-2)

3. George Maroulis and Theodore Simos, Editors
   In the Frontiers of Computational Science
   Lecture Series on Computer and Computational Sciences, Vol 3.
   VSP Brill, Leiden (2005) (ISBN 90-6764-442-0).

4. Theodore Simos and George Maroulis, Editors
   Advances in Computational Methods in Sciences and Engineering 2005
   Lecture Series on Computer and Computational Sciences, Vol 4, Part A and Part B.
   VSP Brill, Leiden (2005) (ISBN 90-6764-441-2).

5. George Maroulis
   Clusters: From a few atoms to nanoparticles.
   Lecture Series on Computer and Computational Sciences, Vol 5.
   VSP Brill, Leiden (2006) (ISBN10 90-6764-456-0).

6. George Maroulis
   Atoms, molecules and clusters in electric fields: Theoretical approaches to the calculation of electric polarizability.
   Imperial College Press (2006) (ISBN 1-86094-676-3).

7. George Maroulis and Theodore Simos, Editors
   Trends and perspectives in modern Computational Science
   Lecture Series on Computer and Computational Sciences, Vol 6.
   VSP Brill, Leiden (2006) (ISBN 90 04 15541 4).

8. Theodore Simos and George Maroulis, Editors
   Recent Progress in Computational Sciences and Engineering
   Lecture Series on Computer and Computational Sciences, Vol 7, Part A and Part B.
   VSP Brill, Leiden (2006) (ISBN 90 04 15542 2).

9. George Maroulis and Theodore Simos, Editors
   Theory and Computation. Old problems and New Challenges
   AIP Conference Proceedings 963, Vol 1 (2007).
   American Institute of Physics (ISBN: 978-0-7354-0477-9).

10. Theodore Simos and George Maroulis, Editors
    Computation in Modern Science and Engineering: Proceedings of the International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007)
    AIP Conference Proceedings 963, Vol 2 PARTS A and B (2007).
    American Institute of Physics (ISBN**:**978-0-7354-0478-6).

11. Theodore Simos, George Maroulis, George Psihoyios and Ch. Tsitouras, Editors
    Selected papers from ICNAAM and ICCMSE 2007
    AIP Conference Proceedings 1046 (2008)
    American Institute of Physics (ISBN 978-0-7354-0574-5)

12. George Maroulis and Theodore Simos, Editors
    Advances in Computational Science
    AIP Conference Proceedings 1108 (2009)
    American Institute of Physics (ISBN 978-0-7354-0644-5)

13. Theodore Simos and George Maroulis, Editors
    Advances in Computational Science Vol. 2
    AIP Conference Proceedings 1148 (2009)
    American Institute of Physics (ISBN 978-0-7354-0685-8)

14. G. Maroulis, T. Bancewicz, B. Champagne and A.D. Buckingham
    Atomic and Molecular Nonlinear Optics: Theory, Experiment and Computation
    A homage to the pioneering work of Stanislaw Kielich (1925-1993)
    IOS Press, Amsterdam, 2011(**ISBN:** 978-1-60750-741-3)

15. T.H.Simos and G.Maroulis, Editors.
    International Conference of Computaional Methods in Science and Engineering 2009 (Rhodes, Greece, 29 September – 4 October 2009)
    AIP Conference Proceedings 1504 (2012)
    American Institute of Physics (ISBN 978-0-7354-1122-7)

Guest Editor. Special issues in Scientific Journals

Special issue **Computational aspects of electric polarizability calculations: Atoms, Molecules and Clusters**.
A collection of 37 papers by a total of 102 authors.
Journal of Computational Methods in Science and Engineering, Vol 4, Nos 3 and 4 (2004).

Special issue **Clusters: From a few atoms to nanoparticles**
Computing Letters 1, issue 4 (2005).

Special Issue **Electric and magnetic properties of atoms and molecules. A special issue in honour of Professor A.D.Buckingham**
(with M.G.Papadopoulos and B.Champagne)
Computing Letters 3, Issues 3-4 (2007).

Special issue **Silicon clusters: Problems, challenges and perspectives**
(with A.Zdetsis)
Journal of Computational Methods in Science and Engineering 7, Issues 3-4 (2007).

Special issue **The challenge of alkali metal clusters. Structure, properties and reactivity**
(with P.Calaminici)
Journal of Computational Methods in Science and Engineering 7, Issues 5-6 (2007).

Special issue **Atomic and Molecular Nonlinear Optics: Theory, Experiment and Computation. A homage to the pioneering work of Stanislaw Kielich (1925-1993)**
Journal of Computational Methods in Science and Engineering 10, Issues 4-6 (2010)

Conferences – Symposia - Colloquia

1. G.Maroulis

Theoretical descriptions of molecular systems.

Annual meeting of the Theoretical Chemists of Eastern Canada, November 1983, Queen's University, Kingston, Ontario.

2. G.Maroulis

Electrical Properties of N_2 by fourth-order many-body perturbation theory.

Annual Fall Meeting, Canadian Association of Physicists, Division of Atomic and Molecular Physics, October 23-24 (1987), University of New Brunswick, Fredericton, New Brunswick.

3. G.Maroulis

Fourth-order MPPT studies of polarizabilities and hyperpolarizabilities.

Atlantic Theoretical Chemistry Symposium, May 12-14 (1988), University of New Brunswick, Fredericton, New Brunswick.

4. G.Maroulis

Reduction of dimensionality, pattern recognition and clustering in spaces of theoretical descriptions of molecules.

1990 CIC (Canadian Insitute of Chemistry) Congress, The Frontiers of Theoretical Chemistry, July 15-20 (1990), Dalhousie University, Halifax, Nova Scotia.

5. G.Maroulis

Trends in Quantitative Structure-Physical Property Relationships.

BIOMED 93. Aminoacids-peptides-proteins. Drug discovery and design. University of Patras, October 14-15 (1993).

6. G.Maroulis

Computational aspects of the calculation of electron correlation corrections for molecular properties: Evaluation of the performance of methods.

Invited Speaker.
8th International Congress of Quantum Chemistry. Satellite Meeting, Smolenice, Bratislava, June 14-18 (1994). Electron correlation in atoms and molecules. New methods and applications.

7. G.Maroulis

Computational aspects of interaction hyperpolarizability calculations.

Invited Speaker.
79th CIC (Canadian Institute of Chemistry) Conference and Exhibition. Memorial University of Newfoundland, St. John's, Newfoundland, June 23-26 (1996).

8. D.Xenides and G.Maroulis

From atoms to clusters: Electric dipole polarizability and hyperpolarizability for P, P_2 and P_4.

34th Symposium for Theoretical Chemistry. September 20-24, 1998, Gwatt-Zentrum at Lake Thun, Switzerland.

9. G.Maroulis

Electric polarizability and hyperpolarizability of H-C≡C-X (X=F,Cl,Br,I).

34th Symposium for Theoretical Chemistry. September 20-24, 1998, Gwatt-Zentrum at Lake Thun, Switzerland.

10. G.Maroulis

Trends and perspectives in electric hyperpolarizability calculations

Invited Speaker.
218th **American Chemical Society** Meeting, New Orleans, August 22-26, 1999.
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 1999, Vol 218, Iss AUG, pp 36.

11. G.Maroulis and D.Xenides

Basis set and electron correlation effects in electric polarizability and hyperpolarizability calculations for O_3, SO_2, SeO_2 and TeO_2.

218th **American Chemical Society** Meeting, New Orleans, August 22-26, 1999.
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 1999, Vol 218, Iss AUG, pp 131.

12. G.Maroulis and P.Karamanis
Hyperpolarizability of C_2X_4 (X=H, F, Cl, Br and I).
218th **American Chemical Society** Meeting, New Orleans, August 22-26, 1999.
ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY 1999, Vol 218, Iss AUG, pp 133.

13. U.Hohm and G.Maroulis
Measurement and theoretical refinements of the polarizability anisotropy of CO_2.
S.-L.Zhang and B.-F.Zhu (Editors)
Proceedings of the XVIIth Conference on Raman Spectroscopy, pp. 86-87.
Wiley, London (2000).

14. U.Hohm and G.Maroulis
Depolarized collision-induced Raman scattering of tetrahedral molecules at elevated temperatures: P_4 and CBr_4.
S.-L.Zhang and B.-F.Zhu (Editors)
Proceedings of the XVIIth Conference on Raman Spectroscopy, pp. 88-89.
Wiley, London (2000).

16. A.Haskopoulos and G.Maroulis*
Interaction dipole moment of the weakly bound complexes of carbon dioxide with rare gases.
XXV European Congress on Molecular Spectroscopy, Coimbra, Portugal, 2000.

17. D.Xenides and G.Maroulis*
Electric multipole moments for SO_2, SeO_2, TeO_2 and the open and closed forms of S_3, Se_3 and Te_3.
XXV European Congress on Molecular Spectroscopy, Coimbra, Portugal, 2000.

18. P. Karamanis and G.Maroulis*
First and second dipole hyperpolarizability of monosubstituted diacetylenes H-C≡C-C≡C-X
CHITEL 2001, Toulouse, France, 2001.

19. A. Chrissanthopoulos, P. Karamanis and G. Maroulis*
Electric dipole moment, polarizability and hyperpolarizability of AlH, AlF and AlCl.
CHITEL 2001, Toulouse, France, 2001.

20. G.Maroulis
Nonlinear polarizability of substituted diacetylenes
Invited Speaker
CHITEL 2001, Toulouse, France, 2001.

21. U.Hohm and G.Maroulis
Collision-induced light scattering of adamantine, $C_{10}H_{16}$ in the gas phase
XVIIIth Conference on Raman Spectroscopy,
Budapest, Hungary, 2002.

22. G.Maroulis
Electric hyperpolarizability: Perspectives and applications in the study of weakly bonded molecules, clusters and molecules with enhanced nonlinear optical properties.
Invited speaker
19th Panhellenic Conference on Chemistry
The many faces of Chemistry and its applications.
Heraklion, Crete, 2002.

23. P.Karamanis and G.Maroulis
Ab initio study of the electric properties of $(CN)_2$. Effect of the relative orienation of the two moieties on the electric (hyper)polarizability of the dimer.
19th Panhellenic Conference on Chemistry
The many faces of Chemistry and its applications.
Heraklion, Crete, 2002.

24. P.Karamanis and G.Maroulis

Electronic structure and electric properties of substituted diacetylenes, H-C≡C-C≡C-X, X = F, Cl, Br, I, CN, NC, CP, PC, Li, Na, K. A systematic study of the effect of substitution on the electric properties .

19th Panhellenic Conference on Chemistry
The many faces of Chemistry and its applications.
Heraklion, Crete, 2002.

25. A.Haskopoulos and G.Maroulis

A systematic study of the the complexes N_2···Rg, Rg = He, Ne, Ar, Kr και Xe. Molecular geometry, dipole moment and polarizability.

19th **Panhellenic Conference on Chemistry**
The many faces of Chemistry and its applications.
Heraklion, Crete, 2002.

26. G.Maroulis

Electric hyperpolarizability calculations

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)
September 12-16, Kastoria, Greece.
T.E.Simos (Editor)
Computational Methods in Sciences and Engineering 2003, pp 400-404
World Scientific, Singapore (2003).

27. A.Haskopoulos and G.Maroulis

Intermolecular interactions of $(H_2O)_2$.

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)
September 12-16, Kastoria, Greece.
T.E.Simos (Editor)
Computational Methods in Sciences and Engineering 2003, pp 223-227
World Scientific, Singapore (2003).

28. N.Karatsis and G.Maroulis

Molecular structure and electric polarizability in sodium chloride clusters.

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)
September 12-16, Kastoria, Greece.
T.E.Simos (Editor)
Computational Methods in Sciences and Engineering 2003, pp 289-291
World Scientific, Singapore (2003).

29. P.Karamanis and G.Maroulis

Electric properties of substituted diacetylenes

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)
September 12-16, Kastoria, Greece.
T.E.Simos (Editor)
Computational Methods in Sciences and Engineering 2003, pp 285-288
World Scientific, Singapore (2003).

30. P. Karamanis, G. Maroulis and C. Pouchan

Size and electric dipole (hyper)polarizability in small $(CdS)_n$ and $(CdSe)_n$ clusters.

COST ACTION 26
Development of Density Functional Theory models for an accurate description of electronic properties of materials possessing potential high non-linear optical properties
Paris 9-11 January (2004).

31. Anastasios Haskopoulos and George Maroulis

A paradigmatic study of the electric (hyper)polarizability of small copper clusters.

COST ACTION 26
Development of Density Functional Theory models for an accurate description of electronic properties of materials possessing potential high non-linear optical properties
Paris 9-11 January (2004).

32. G.Maroulis

Theoretical prediction of electric hyperpolarizabilities of small metal clusters. A systematic study of conventional ab initio and DFT calculations.

COST ACTION 26
Development of Density Functional Theory models for an accurate description of electronic properties of materials possessing potential high non-linear optical properties
Paris 9-11 January (2004).

33. G.Maroulis

Computational strategies for the determination of the electric (hyper)polarizability of calcium clusters: Ca_4 as a test case with some preliminary results on Ca_7.

COST ACTION 26
Development of Density Functional Theory models for an accurate description of electronic properties of materials possessing potential high non-linear optical properties
Pau 24-26 September (2004).

34. G.Maroulis and A.Haskopoulos

Electric hyperpolarizability of small copper clusters. The tetramer Cu_4 as a test case

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2004)
November 19-23, Vouliagmeni (Attica), Greece.
T.E.Simos and G.Maroulis (Editors)
International Conference of Computational Methods in Sciences and Engineering 2004
Lecture Series on Computer and Computational Sciences Vol 1, pp 1096-1100
VSP Brill, Leiden (2004).

35. A.Haskopoulos and G.Maroulis

Interaction dipole moment and (hyper)polarizability in Rg-Xe

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2004)
November 19-23, Vouliagmeni (Attica), Greece.
T.E.Simos and G.Maroulis (Editors)
International Conference of Computational Methods in Sciences and Engineering 2004
Lecture Series on Computer and Computational Sciences Vol 1, pp 1077-1080.
VSP Brill, Leiden (2004).

36. A.Hatzis, A.Haskopoulos and G.Maroulis

A database of gaussian-type basis sets applied to the calculation of electric properties of the azide anion.

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2004)
November 19-23, Vouliagmeni (Attica), Greece.
T.E.Simos and G.Maroulis (Editors)
International Conference of Computational Methods in Sciences and Engineering 2004
Lecture Series on Computer and Computational Sciences Vol 1, pp 1081-1084
VSP Brill, Leiden (2004).

37. C.Makris and G.Maroulis

Electric properties of F2, ClF, BrF and IF.

International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2004)
November 19-23, Vouliagmeni (Attica), Greece.
T.E.Simos and G.Maroulis (Editors)
International Conference of Computational Methods in Sciences and Engineering 2004
Lecture Series on Computer and Computational Sciences Vol 1, pp 1092-1095
VSP Brill, Leiden (2004).

38. P.Karamanis and G.Maroulis

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