

Curriculum Vitae

Name: Giannoula Theodorakopoulos

Year of birth: 1951

Family status: married, 4 children

Home address: Roumelis St. 14, Athens 118 52, Greece. **Tel.** +30-10-3421927

Work address: Theoretical and Physical Chemistry Institute, The National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece. **Tel.:** +30-10-7273-800, **Fax:** +30-7273-794, **email:** ithe@eie.gr

Position: Researcher A (Director of Research).

Education: All university and post-graduate studies at University of Toronto, Toronto, Canada.

Degrees: B. Sc. in 1973 (Physical Chemistry), M. Sc. in 1974 (Theoretical Chemistry) and Ph. D. In 1978 (Theoretical Chemistry).

Theses: M. Sc. Thesis "A theoretical study of the conformational rigidity of the thiothiophthenes". Supervisor: Prof. I. G. Csizmadia

Ph. D. Thesis "A theoretical study on the energetics of molecular ionization". Supervisor: Prof. I. G. Csizmadia

Fellowships:

EC Human capital and mobility category 40 fellowship, 1/8/94 - 31/7/95,
National Research Council of Canada, Post-Doctoral (NATO) Fellowship, 1978-1980,
National Research Council of Canada, Post-Graduate Scholarship, 1975-78,
University of Toronto Open fellowship, 1974-75,
Ontario Scholar 1969.

Teaching experience: 1) Sessional lecturer (while on Sabbatical) at the Chemistry Department of Carleton University, Sept. -Dec. 1987. Fourth year group theory course, CHEM 410.

2) Teaching Assistant (Chemistry Department, University of Toronto): Sept. 1973 – May 1978, in Physical Chemistry courses.

Administrative experience: Member of the advisory scientific council of the TPCI from 1988-present.

Research experience: I have a permanent research position at the Theoretical and Physical Chemistry Institute of the National Hellenic Research Foundation (TPCI/NHRF) from May 1973-present: Scientific Collaborator from May 1 1978 to April 30 1984, Researcher C from May 1 1984 to Dec. 31 1989, Researcher B from Jan.1 1990 to March 31, 1998 and Researcher A since April 1, 1998.

Visiting positions while on Sabbatical leaves from TPCI/NHRF: at the Chemistry Department University of Toronto, Toronto, Canada, August 2002-July 2003, Oxford University, Oxford England, August 1993- July 1994 and at Carleton University, Ottawa Canada, August 1987- July 1988. Several long visits of

duration 1-5 months to Bonn University (1979-1982) and to Wuppertal University (1983-present).

Research interests:

Development and applications of theoretical methods for investigations of structure and processes in excited and highly excited states of small molecules. This work finds applications in the atmospheric chemistry, the chemistry of interstellar space, in the design of systems for energy storage and energy transfer as well as for the design of laser systems.

Current research interests include:

(i) Investigation by theoretical quantum mechanical methods, semiempirical and density functional of reactions of molecules on semiconductor surfaces leading to imprinting of molecular structure on the surfaces (e.g. C₆H₆ and Cl or Br -substituted benzene on Si(111)7X7). (ii) theoretical study of functionalized carbon nanohorns and fullerene hybrids.

External funding projects:

- Member of team (I.D. Petsalakis, G. Theodorakopoulos and N. Tagmatarchis) involved in NANOHOST project (FP7-REGPOT-2007-1) starting Feb. 1,2008
- Greece-Slovakia joint research and technology project Theoretical investigation of group III metal nitrides and their chemisorption on Si(111). Formation of thin films, nanowires and nanoclusters, 2004-2006 but in fact 2005-2007.
- Scientist in charge of MCIF-EU (Excited states of Molecules adsorbed on Metal Clusters), 2003-2004
- NATO PST/CLG.978504, "Theoretical study of the spectroscopy of polyatomic molecules containing alkaline earths", 2002-2003,
- Greece-Poland joint research and technology project 2001-2003, Theoretical study of the spectroscopy of polyatomic molecules containing alkaline earth atoms (project coordinator),
- Greece-Poland joint research and technology project 2001-2003, "Development of a theoretical method for the study of interactions between open-shell molecular units. Applications to moieties containing transition metals".
- INTAS 1999, 'Multi-vectors correlations in gas phase chemistry', 2000-2003, (project coordinator).

Collaborations

1. University of Toronto Canada (The Honourable J.C.Polanyi, PC,CC,FRS)
2. Wuppertal University Germany (R.J. Buenker, Prof.)
3. Oxford University England (M. S. Child, Prof.,FRS)
4. Lam Research Corporation California U.S.A (J.Luque, Dr.)
5. Institute of Physical and Theoretical Chemistry, Wroclaw University of Technology, Poland (S.Rozsak, Prof.)

6. Department of Chemistry, Adam Mickiewicz University, Poland.(Jacek Koput, Prof.)
7. Wilfried Laurier University Waterloo Canada (I.P.Hamilton, Prof.)
8. St. Petersburg State University, Department of Optics and Spectroscopy Russia (A.Devdariani, Prof.and G.Gerasimov, Prof.)
9. N.N.Semenov Institute of Chemical Physics, Russian Academy of Sciences, Russia (G.Golubkov, Prof.)
10. Max Planck Institute for Quantum Optics, Garching Germany (H.Figger Dr.)
11. Comenius University, department of Physical and Theoretical Chemistry (M. Miro, Prof.)

Participation in international conferences

- VI International Symposium on Organic Sulphur Chemistry, Bangor, North Wales, July 1-5, 1974
- Second International congress on Quantum Chemistry, New Orleans, La., U.S.A., April 19-24, 1976
- Theoretical Organic Chemistry Summer School and Symposium, Teneriffe, Canary Islands, Spain, June 13-27, 1976
- NATO Advanced Study Institute on Excited States in Quantum Chemistry, Cos, Greece, June 4-18, 1978
- NATO Advanced Study Institute on Potential Energy Surfaces, Menton, France, July 4-10, 1978
- NATO Advanced Study Institute on Molecular Ions, Cos, Greece, October 5-18, 1980
- Sanibel Symposium, Palm Coast, Florida, U. S. A., March 10-15, 1979
- Seventh Canadian Symposium on Theoretical Chemistry, Banff, Alberta, Canada, June 15-20, 1980
- Workshop of Far U.V. Spectroscopy and Photochemistry, Mulheim am Ruhr, W. Germany, February 24-26, 1981
- Discussion Meeting on Calculation of correlated Wavefunctions with applications involving Non-Adiabatic and Relativistic Effects, Bad Münstereifel, W. Germany, Feb. 27- March 3, 1983
- 5-th International Congress on Quantum Chemistry, Montreal, Canada, August 18- 24, 1985
- Satellite symposium on molecular structure and chemical reactivity. Toronto, Ontario, Canada, August 25-28, 1985
- Regional Symposium on Chemical Reactivity, Waterloo, Ontario, Canada, October 24- 26, 1987
- The third Chemical Congress of North America, Toronto, Ontario, Canada. June 5-10, 1988
- International Symposium on Electronic Structure and Properties of molecules and Crystals, Cavtat, Yugoslavia, Aug. 29-Sept.3 1988
- WATOC 93 , Toyohashi, Japan, July 18-24, 17. CCP6 Workshop, Intramolecular Dynamics in the Frequency and Time Domains. 15-16 December 1994, St. Edmund Hall, Oxford, England.
- Royal Society Discussion Meeting on Molecular Rydberg Dynamics.

6-7 November 1996, 6 Carlton House Terrace, London, England.

- International Seminar on Physics of Electronic and Atomic Collisions, Klyasma, Moscow region, Russia, March 12-16, 2001.
- International Seminar on atomic interactions and differential scattering, St. Andreasberg, Germany, 18-21 March 2002.
- 12th International Conference on Scanning Tunneling Microscopy/Spectroscopy and Related Techniques, July 21-25, 2003, Eindhoven University of Technology, Eindhoven, the Netherlands
- Ein Gedi Workshop II, Non Adiabatic Processes at Surfaces, Ein Gedi, Israel January 11-15 2004.

Invited talks

- Institute of Physical Chemistry, Bonn University, November 1979, on “FOTOS in molecules”.
- Max-Planck Institute in Stuttgart, Germany, Νοέμβριος 1979, on “FOTOS in molecules”.
- Department of Physics, University of Guelph, Canada, Δεκέμβριος 1987, “Diatomic Rydberg Molecules”.
- Research Centre FOR, Crete, Greece, October 1989, on “Rydberg “Molecules”.
- Max-Planck Institute for Quantum Optics, Garching, Germany, February 1994, on “Rydberg Molecules”.
- Department of Theoretical Chemistry, Oxford University, November 1994, on “Ab initio calculations on Rydberg Molecules”.
- Theoretical Chemistry Department, Wuppertal University, July 2000, on “Ab initio and MQDT methods for the theoretical study of Rydberg spectra.
- Theoretical Chemistry Department, Wuppertal University, March 2002 “Ab initio calculations on the potential energy surfaces of polyatomic molecules containing alkaline earths”
- Rutherford Appleton Laboratory, Didcot-Oxford England, November 2007, “Calculations on excited electronic states of small molecules and larger systems”.
- Ein Gedi Workshop II, Non Adiabatic Processes at Surfaces, Ein Gedi, Israel January 11-15 2004. “Theoretical study of reactions of benzene and dibromobenzene at a Si(111) surface”.

Giannoula Theodorakopoulos, publication list

1. P.G. Mezey, A. Kucsman, G. Theodorakopoulos and I. G. Csizmadia, Theoretical conformation analysis of a simple sulphilimine model, *Theoret. Chim. Acta (Berl.)* **38**, 115 (1975).
2. O.P. Strausz, L. Gammie, G. Theodorakopoulos, P.G. Mezey, and I.G. Csizmadia, The ground state of silaethylene. An *Ab Initio* molecular orbital study of the lower electronic manifold, *J. Am. Chem. Soc.*, **98**, 1622 (1976).
3. G. Theodorakopoulos, I.G. Csizmadia, M.A. Robb, A. Kucsman and I. Kapovits, Experimental (ESCA) and theoretical (SCF-MO) determination of the oxidation state of sulphur in bis(2-

- carboxy phenyl) sulphur dihydroxide dilactone, J. Chem. Soc. Faraday Transactions II, 73, 293 (1977).
4. S. C. Nyburg, G. Theodorakopoulos and I. G. Csizmadia, Conformations of thiathiophthenes and related molecules, Theoret. Chim. Acta (Berl.) 45, 21 (1977).
 5. I. G. Csizmadia, G. Theodorakopoulos, H. B. Schlegel, M.H. Whangbo and S. Wolfe, The balance between electronic and nuclear energy in conformational change, Can. J. Chem. 55, 986 (1977).
 6. G. Theodorakopoulos, M. A. Robb and I. G. Csizmadia, A theoretical study on the molecular ionization potentials of selected sulphur compounds, in Progress in Theoretical Organic Chemistry, vol. 2, I. G. Csizmadia editor, Elsevier Scientific Publishing Company, Amsterdam 1977.
 7. S. C. Nyburg and G. Theodorakopoulos, Experimental and theoretical studies on the conformational rigidity of thiathiophthene and related molecules, in Progress in Theoretical Organic Chemistry vol. 2, I. G. Csizmadia editor, Elsevier Scientific Publishing Company, Amsterdam, 1977.
 8. O. P. Strausz, M. A. Robb, G. Theodorakopoulos, P. G. Mezey and I. G. Csizmadia, Calculations on the Singlet-triplet energy separation of silaethylene, Chem. Phys. Lett. 48, 162 (1977).
 9. R. Eade, M. A. Robb, G. Theodorakopoulos and I. G. Csizmadia, Calculation of sulphur L(S_{2p})—MM' Auger energies of H₂S, Chem. Phys. Lett. 52, 526 (1977).
 10. P. G. Mezey, K. Yates, G. Theodorakopoulos and I. G. Csizmadia, Uniform quality Gaussian bases for organo-silicon compounds, Internat. J. Quant. Chem. 12, 257 (1977).
 11. O. P. Strausz, C. Kozmutza, E. Kapuy, M. A. Robb, G. Theodorakopoulos and I. G. Csizmadia, Vertical proton affinities of CH₂O and CH₂OH⁽⁺⁾ in their ground singlet, excited triplet and ionized doublet states, Theoret. Chim. Acta 48, 215 (1978).
 12. M. A. Robb, G. Theodorakopoulos and I. G. Csizmadia, Theoretical Auger energies using a frozen orbital approximation. The sulphur 2p—mm' and the oxygen 2s—mm' Auger spectra of SO₂, Chem. Phys. Lett. 57, 423 (1978).
 13. O. P. Strausz, R. K. Gosavi, G. Theodorakopoulos and I. G. Csizmadia, A preliminary investigation on the thermodynamic stability of triplet carbenoid isomers of silaethylene, Chem. Phys. Lett. 58, 43 (1978).
 14. G. Theodorakopoulos, C. A. Nicolaides and D. R. Beck, One-electron Binding and Auger energies of sulphur in atomic and molecular states, Int. J. Quant. Chem. Symp. 13, 671 (1979).
 15. G. Theodorakopoulos, M. A. Robb, and I. G. Csizmadia, Theoretical investigation of the chemical shifts of the K—LL' Auger energies for a series of sulphur compounds, Chem. Phys. Lett. 69, 66 (1980).
 16. C. A. Nicolaides and G. Theodorakopoulos, FOTOS applied to molecules: Oscillator strengths in H₂O. Int. J. Quant. Chem. Symp. 14, 315 (1980).
 17. G. Theodorakopoulos, A. Kucsman, I. Kapovits, G. Naray-Szabo, and I. G. Csizmadia, Minimal basis study of inner-shell ionization potentials for molecules containing Sulphur: S,S- Diphenyl-N-p-Tolylsulfonyl-Sulphilimine, J. Comput. Chem. 2, 212 (1981).
 18. G. Theodorakopoulos, S. D. Peyerimhoff and R. J. Buenker, *Ab initio* configuration interaction study of the X³Σ⁻, a¹Δ and b¹Σ⁺ states of SO and S₂, Chem. Phys. Lett. 81, 413 (1981).
 19. G. Theodorakopoulos, C. A. Nicolaides, R. J. Buenker and S. D. Peyerimhoff, Potential energy surfaces for the photodissociation H₂O — O (¹D) + H₂ (¹Σ_g⁺), Chem. Phys. Lett. 89, 164 (1982).
 20. S. C. Farantos, G. Theodorakopoulos and C. A. Nicolaides, A non-Van der Waals minimum of the He(¹S) + H₂(B¹Σ_u⁺) excited surface, Chem. Phys. Lett. 100, 263 (1983).
 21. G. Theodorakopoulos, S. C. Farantos, R. J. Buenker and S. D. Peyerimhoff, MRD-CI calculations on the potential energy curves of the ground and excited electronic states of the noble-gas hydrides, HeH, NeH, and ArH, J. Phys. B. 17, 1453 (1984).

22. C. A. Nicolaides, G. Theodorakopoulos and I. D. Petsalakis, Theory of Chemical Reactions of vibronically excited H_2 . Prediction of a strongly bound H_4 excited state, *J. Chem. Phys.* **80**, 1705 (1984).
23. G. Theodorakopoulos, I. D. Petsalakis, R. J. Buenker and S. D. Peyerimhoff, MRD-CI calculations on the bending potentials of H_2O in the ground and in excited states, *Chem. Phys. Lett.* **105**, 253 (1984).
24. C.A.Nicolaides, I.D.Petsalakis and G.Theodorakopoulos, Theory of chemical reactions of vibronically excited $H_2(B^1\Sigma_u^+)$ III. Formation of bound excited states of the $(H_2)_2$, $(H_2)_3$ and $(H_2)_5$ clusters, *J. Chem. Phys.* **81**,748(1984).
25. I.D.Petsalakis, G.Theodorakopoulos, C.A.Nicolaides, R.J.Buenker and S.D.Peyerimhoff, Nonorthonormal CI for molecular excited states. I. The sudden polarization effect in 90° twisted ethylene, *J. Chem. Phys.* **81**,3161(1984).
26. G.Theodorakopoulos, I.D.Petsalakis, I.G.Csizmadia and M.A.Robb, Theoretical and experimental ionization potentials of $(CH_3)_2S$ and $(CH_3)_2SO$. The effect of substituents R on the sulphur ESCA shifts in the series R_2S , R_2SO , R_2S , *J. Molec. Struct.* **110**,381(1984).
27. I.D.Petsalakis, G.Theodorakopoulos, C.A.Nicolaides and R. J. Buenker, Nonorthonormal CI for molecular excited states. II. The zwitterionic states of terminally twisted butadiene. *J. Chem. Phys.* **81**,5952(1984).
28. G.Theodorakopoulos, I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, The $X^1A_1 - A^1B_1$ transition moment of H_2O using State-Specific Configuration Interaction wavefunctions. *J. Chem. Phys.* **82**,912(1985).
29. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker, MRD-CI calculations on the asymmetric stretch potentials of H_2O in the ground and the first seven singlet excited states. *Chem. Phys.* **96**,217(1985)
30. G.Theodorakopoulos, I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, Configuration interaction study of the oscillator strengths for the $B^1A_1 - X^1A_1$ and $D^1A_1 - X^1A_1$ transitions of the water molecule, *Chem. Phys.* **100**,331(1985).
31. G.Theodorakopoulos, I.D.Petsalakis and C.A.Nicolaides, A method for the calculation of transition moments between electronic states of molecules using a different one-electron basis set for each state, *Inter. J. Quantum Chem.* **29**,399(1986).
32. G.Theodorakopoulos, I.D.Petsalakis and C.A.Nicolaides. Potential energy hypersurfaces of H_4 in the ground and the first two singlet excited electronic states. *J. Molec. Struct.* **149**,23(1987).
33. G.Theodorakopoulos, I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, Nonorthonormal basis calculations of the transition moment for the Phillips system ($A^1\Pi_u - X^1\Sigma_g^+$) in C_2 . Theoretical lifetime of the $A^1\Pi_u$ state. *Chem. Phys.* **112**,319(1987).
34. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker. states of H_2O along a linear dissociation path leading to $OH+H$. *Chem. Phys. Lett.* **138**,71(1987).
35. G.Theodorakopoulos, I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, Theoretical dipole transition moments for the transitions to the ground state $X^2\Sigma^+$ from the $A^2\Sigma^+$, $B^2\Pi$, $C^2\Sigma^+$, $D^2\Sigma^+$ and $E^2\Pi$ states and the $B^2\Pi - A^2\Sigma^+$ system in HeH , *J. Phys. B: At. Mol. Phys.* **20**,2339(1987).
36. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker, Theoretical investigation of the excited states of NeH : Calculations of dipole transition moments and radial coupling matrix elements, *J. Phys. B: At. Mol. Phys.* **20**,5335(1987).
37. I.D.Petsalakis, G.Theodorakopoulos, C.A.Nicolaides and R.J.Buenker, Theoretical dipole transition moments for transitions between bound electronic states and non-adiabatic coupling matrix elements between $2\Sigma^+$ states of HeH , *J. Phys. B: At. Mol. Phys.* **20**,5959(1987).
38. I.D.Petsalakis, G.Theodorakopoulos, J.S.Wright and I.P.Hamilton, The Rydberg states of FH_2 , *J. Chem. Phys.* **88**,7633(1988).

39. G.Theodorakopoulos, I.D.Petsalakis, and R.J.Buenker. Non-adiabatic interactions between the C $2\Sigma^+$ and D $2\Sigma^+$ electronic states of HeH, Chem. Phys. Lett. 148,285(1988).
40. G.Theodorakopoulos and I.D.Petsalakis, Ab initio calculations on the ground and excited electronic states of KrH.Chem.Phys. Lett. 149,196(1988).
41. I.D.Petsalakis, G.Theodorakopoulos and R.J.Buenker, Radiative dissociation and predissociation in HeH and NeH: A theoretical treatment using square-integrable functions. Phys. Rev. A 38,4004(1988).
42. I.D.Petsalakis, G.Theodorakopoulos, J.S.Wright and I.P.Hamilton, Electronic and vibrational calculations of the $2^2A_1(3p) \rightarrow 1^2B_2(3p)$ and the $3^2A_1(4s) \rightarrow 1^2B_2(3p)$ transitions in FH₂ and FD₂. J.Chem. Phys. 89,6841 (1988).
43. I.D.Petsalakis, G.Theodorakopoulos and J.S.Wright, Theoretical calculations on electronic transitions for H₃, including Rydberg and transition state spectra. J. Chem. Phys. 89, 6850 (1988).
44. P.Karafiloglou, G.Theodorakopoulos and I.D.Petsalakis,Valence bond analysis of molecular orbital wavefunctions. The ionicity of the B $1\Sigma_u^+$ state of H₂. J. Molec. Struct. THEOCHEM 180,31 (1988).
45. I.D.Petsalakis and G.Theodorakopoulos, Theoretical calculations on radiative and nonradiative processes of quartets states of HeH, Chem. Phys. 130,211 (1989).
46. I. D. Petsalakis, G. Theodorakopoulos, and V. Barcklay, Theoretical calculations on the ground electronic state of NeHe⁺, Chem. Phys. Letters 160,189(1989).
47. G. Theodorakopoulos, I.D. Petsalakis, R.J. Buenker and M.Honigmann, Theoretical calculations on the radiative lifetime of the A² Σ^+ state of CH, Chem. Phys. 137,137 (1989).
48. I. D. Petsalakis, A. Metropoulos, G. Theodorakopoulos, and C. A. Nicolaides , An estimate of the lifetime of excited tetrahydrogen, Chem. Phys. Lett. 158,229 (1989).
49. I.D. Petsalakis, G. Theodorakopoulos, J. S. Wright and I. P. Hamilton, Potential energy surface for large-amplitude motion and vibrational spacing for FH₂⁺.J.Chem.Phys.92, 2440 (1990).
50. I. D. Petsalakis, G. Theodorakopoulos and R. J. Buenker, Theoretical treatment of predissociation in the A² Σ^+ , B² Π and C² Σ^+ states of HeH. J. Chem. Phys.92 4920 (1990)
51. I. D. Petsalakis, T. Merkouris, G. Theodorakopoulos and C. A. Nicolaides, Predissociation resonances from a complex eigenvalue Schrödinger equation. J. Phys. B.23, L89(1990)
52. I.D. Petsalakis, Th. Mercouris, G. Theodorakopoulos and C. A. Nicolaides, Distributed Complex Gaussian basis sets: A useful function space for the solution of predissociation problems by the isotope effect of NeH,NeD. J. Chem.Phys. 93,6642(1990).
53. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker, Theoretical calculations of the Rydberg spectra of ArH, Molec.Phys. 71, 1055 (1990)
54. G. Theodorakopoulos and I.D.Petsalakis, Theoretical Study of CH₂⁺ J.Mol.Struct.(Theochem) 230 205 (1991)
55. G. Theodorakopoulos and I.D.Petsalakis, Asymmetric dissociation and bending potentials of H₂S in the ground and excited electronic states, Chem.Phys.Lett. 178, 475 (1991).
56. I. D. Petsalakis, Th. Mercouris, G. Theodorakopoulos and C.A. Nicolaides, Theory and ab-initio calculations of partial widths and interchannel coupling in predissociating diatomic states. Application to HeF. Chem.Phys.Lett. 182, 561 (1991)
57. I. D. Petsalakis, G. Theodorakopoulos, C. A. Nicolaides and R.J.Buenker, Nearly-diabatic states by maximization of the non-orthonormal overlap between model-diabatic and MRD-CI wavefunctions, Chem.Phys.Lett. 185, 359 (1991)
58. I.D. Petsalakis, G. Theodorakopoulos and S.Consta, Theoretical calculations on the electronic states XeH , Mol.Phys. 75, 805 (1992).
59. I. D. Petsalakis, G. Theodorakopoulos and C.A.Nicolaides, Adiabatic and Quasi-diabatic $2\Sigma^+$ states of BeH, J. Chem.Phys. 97, 7623 (1992).

60. I. D. Petsalakis and G. Theodorakopoulos, Theoretical Calculations on Rydberg states of H₂S, Chem.Phys.Lett. 200, 387 (1992).
61. I. D. Petsalakis and G. Theodorakopoulos, Theoretical lifetimes of Rydberg states of ArH and ArD, J.Phys.B25, 5353 (1992).
62. G. Theodorakopoulos, I. D. Petsalakis and C. A. Nicolaides, Diabatic potentials for the 1¹A" and 2¹A" states of H₂S. Chem. Phys. Lett.207,321(1993).
63. G. Theodorakopoulos and I. D. Petsalakis, Potential energy curves and radiative lifetimes of Rydberg states of NaHe. J.Phys. B26 4367 (1993).
64. I. D. Petsalakis, G. Theodorakopoulos and C. A. Nicolaides, Quasi-diabatic states for intramolecular charge transfer. Application to the protonation of NH₃. J. Chem. Phys. 100, 5870 (1994).
65. G. Theodorakopoulos and I. D. Petsalakis, Rydberg spectra of ArH. Bound-Bound interactions and lifetimes of the Rydberg states. J. Chem.Phys. 101, 194 (1994).
66. J.-ping Gu, G. Hirsch, R. J. Buenker, I. D. Petsalakis, G. Theodorakopoulos and M.-bao Huang, Electronic states and radiative transitions in LiAr, Chem. Phys. Lett. 230, 473 (1994).
67. I. D. Petsalakis and G. Theodorakopoulos, Ion-pair and Rydberg states of ArH. J.Phys. B 27, 4483 (1994).
68. I. D. Petsalakis G. Theodorakopoulos and M.S. Child, Ab initio multichannel quantum defects for the 1A₁ Rydberg states of H₂O. J.Phys. B 28 ,5179 (1995).
69. G. Theodorakopoulos, I.D. Petsalakis and M.S. Child, On the construction and use of ab initio quantum defect functions for H₂O. J. Phys B : At. Mol. Opt. Phys. 29,4543 (1996).
70. I. D. Petsalakis, G. Hirsch, R. J. Buenker and G. Theodorakopoulos, Predissociation widths and lifetimes of the n=3 ²Σ⁺ and ²Π states of BeH and BeD, J. Phys. B. At. Mol. Opt. Phys. 30,4935(1997).
71. G. Theodorakopoulos ,I. D. Petsalakis and M.S. Child, An ab initio potential energy surface and spectroscopic constants for the ground state of NO₂⁺. Journal of Molec. Struct. (Theochem) 434,177(1998).
72. I. D. Petsalakis, G. Theodorakopoulos, Y. Li, G. Hirsch, R. J. Buenker and M. S. Child, Theoretical study on the Rydberg states of NeH. Ab initio quantum defect and complex coordinate calculations. J. Chem. Phys. 108,7607(1998).
73. D. Azinovic, R. Bruckmeier, Ch. Wunderlich, H. Figger, G. Theodorakopoulos and I. D. Petsalakis, Dynamics on the ground state potential surfaces of H₃ and its isotopomers from their UV spectra. Phys. Rev. A 58,1115(1998).
74. M. Honigmann, G. Hirsch, R.J. Buenker, I.D. Petsalakis and G.Theodorakopoulos, Complex coordinate calculations on autoionizing states of HeH and H₂, Chem. Phys. Let. Chem. Phys. Let. 305 465, (1999).
75. I. D. Petsalakis, D. Papadopoulos, G. Theodorakopoulos and R.J. Buenker, Theoretical calculations on the linewidths of rovibrational levels of the 3d Rydberg states of BeH and BeD, J. Phys. B. 32, 3225, (1999).
76. G.Theodorakopoulos, I.D.Petsalakis and I.P.Hamilton, Ab Initio calculations on the ground and excited states of BeOH and MgOH, J.Chem. Phys.111, 10484 (1999)
77. I.D.Petsalakis and G.Theodorakopoulos, Electronic states of CF⁺, Chem. Phys. 254, 181(2000)
78. I.D.Petsalakis, R. J. Buenker, H.-P. Lieberman, A.B. Alekseyev, A.Z. Devdariani and G. Theodorakopoulos, Potential Energy curves and dipole transition moments to the ground state of the system Ar* (3p⁵4s, ³P, ¹P)+Ne, J. Chem. Phys. 113,5812(2000)
79. I. D. Petsalakis, R. J. Buenker, H. -P. Lieberman, R. J. Buenker and G. Theodorakopoulos, Potential energy curves and dipole transition moments for electronic states of ArHe and ArNe. J. Chem. Phys. 115,6365 (2001).
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81. G.Theodorakopoulos, I.D.Petsalakis and M.S.Child, On the construction and use of ab initio quantum defect functions for the Rydberg spectra of molecules. *Rus.J.Phys.Chem.* 76,S95(2002)
82. I.D.Petsalakis, G.Theodorakopoulos and R.J.Buenker, Complex coordinate calculations on predissociating states of diatomic molecules *Russian Journal of Phys.Chem.* 76,S1(2002)
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