

CURRICULUM VITAE

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EDUCATION

Diploma in Physics (BSc.), Aristotelean University of Thessaloniki, Department of Physics, 1980

Ph.D. in Molecular Physics, Kapodistrian University of Athens, Department of Physics and The National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, 1986.

PROFESSIONAL BACKGROUND

Place of permanent employment: Theoretical and Physical Chemistry Institute, The National Hellenic Research Foundation, Athens, Greece.

Positions: Researcher A, Director of research (October 2002 – present)

Researcher B (May 1998 –October 2002)

Researcher C (January 1990 – April 1998)

Researcher D (January 1986- December 1989)

RESEARCH VISITS

(a) Sabbatical leave September 2013 - July 2014

(1) The Fritz Haber Center for Molecular Dynamics and the Chaim Weizmann Chemistry Institute, Hebrew University of Jerusalem, Jerusalem 91904, Israel (September 2013-December 2013)

Collaboration with Prof. Roi Baer on DFT methods exploring charge transfer phenomena.

(2) Chemistry Department, North Carolina State University, 604 Cox Hall, 2700 Stinson Dr., Raleigh NC27695-8204 U.S.A. (January 2014-July 2014)

Collaboration with Prof. J. L. Whitten on theoretical studies on photochemistry of molecules

(b) Sabbatical leave August 2002 - July 2003

Department of Chemistry, University of Toronto, Ontario, 80 George St. M5S3H6, Canada

Collaboration with Prof. J.C.Polanyi (Nobel in Chemistry 1986) on theoretical study of the attachment of molecules on Si(111) surfaces

(c) Bergische Universität – Gesamthochschule Wuppertal, Theoretische Chemie, Fachbereich 9 –Gaussstrasse 20, D-42097 Wuppertal, Germany

From October 1982 – 2002, visits of a few weeks almost every year

Collaboration with Prof. R. J. Buenker and his group on development of computer programs for molecular calculations.

(d) Sabbatical leave August 1994 - July 1995

Department of Theoretical Chemistry, Oxford University, 5 South Parks Rd. Oxford OX1 3UB, England.

Collaboration with Prof. M.S. Child on development of theory and computational program Multi-channel Quantum Defect calculations.

(e) Sabbatical leave August 1987 - July 1988

Department of Chemistry, Carleton University, Ottawa K1S 5B6, Canada.

Collaboration with Prof. J.S. Wright on spectroscopy of Rydberg molecules.

RESEARCH INTERESTS

My research interests lie mainly in the field of molecular physics from a theoretical point of view. Of particular interest are the determination of excited states of molecules as well as the interaction of molecules with electromagnetic radiation. In my work, both development of theoretical methods and applications have been carried out. They are within the framework of Quantum Mechanics and are devoted to

- theoretical studies on donor-acceptor carbon based materials (photovoltaics, photonics)
- theoretical calculations on organic light emitted diodes (OLED)
- theoretical investigations on visually detected molecular sensors (chemical warfare agents, bio-sensors)
- theoretical studies on molecules in confined space
- theoretical investigation of attachment of molecules at Si(111) surface (molecular printing)
- the prediction of the spectra of diatomic and triatomic molecules,
- the calculation of predissociation resonances (Complex coordinate rotation)

- the prediction of highly excited molecular states (Multi-channel Quantum Defect Theory)
- calculations including relativistic effects for molecules with heavy atoms
- time-dependent studies of photodissociation as well as laser-induced molecular formation,
- the calculation of “difficult” electronic states involving near degeneracies and symmetry breaking (Non-orthonormal configuration interaction, Multi-Reference single and Double excitations C. I.)

EXTERNAL FUNDING PROJECTS

European Commission (EC)

- 1.** NANOHOST: Carbon nanohorn-based hybrid materials for energy conversion. Reinforcing and expanding the research potential of carbon-nanostructures laboratory to a regional and European kernel of excellence. EU FP7, Capacities (GA 201729), (2008-2011), N. Tagmatarchis (P.I.), G. Theodorakopoulos, I.D. Petsalakis
- 2.** COPET—Control of photo-induced energy transfer in functionalized carbon nanostructures towards design of nanoscale applications, FP7-PEOPLE- IRG-2008 (2008-2012), G. Theodorakopoulos (PI), I.D. Petsalakis, I. Thanopoulos (research fellow)
- 3.** Excited states of molecules adsorbed on metal clusters, EU/Marie Curie, (2002-2003), G. Theodorakopoulos (PI), I.D. Petsalakis, R.J.Buenker
- 4.** Multivector correlations in gas-phase chemistry, EC/INTAS, (2000-2002), G. Theodorakopoulos (PI), I.D. Petsalakis with partners 8 academic/research organizations
- 5.** Relativistic core potentials calculations on lead halides, EC/MCIF, (2000 - 2001), I.D. Petsalakis

Other Sources

- 1.** Fluorescent sensors for nerve and other warfare agents, NATO, (2009-2011) I.D. Petsalakis (P.I.), G. Theodorakopoulos
- 2.** Theoretical study of the spectroscopy of polyatomic alkaline earth containing molecules, NATO, (2002-2004), G. Theodorakopoulos (P.I.), I.D. Petsalakis
- 3.** Theoretical study of the VUV emission of Kr +Xe, NATO, (2001-2002), I.D. Petsalakis (P.I.), G. Theodorakopoulos
- 4.** Calculations on alkaline earth hydroxides, NATO, (1998-2001) G. Theodorakopoulos (P.I.), I.D. Petsalakis
- 5.** Alexander Von Humboldt Fellowship, Alexander Von Humboldt Foundation, (1995-1996), I.D. Petsalakis

National Sources

1. Interaction of Al clusters with methane. GSRT / EPET-II / PENED '03, (2005-2009), N. Bacalis (PI), I.D. Petsalakis
2. Nanostructured inorganic and organic-inorganic hybrid materials: synthesis, fundamental understanding, and advanced functionality, GSRT (2002-2005), E.I. Kamitsos (PI) and all researchers of TPCI participating.
3. Theoretical investigation of group III metal nitrides and their chemisorption on Si(111). Formation of thin films, nanowires and nanoclusters, GSRT (Greece-Slovakia), (2004-2006), G. Theodorakopoulos (P.I.), I.D. Petsalakis
4. Optimization in business processes, GSRT (PRAXE), (2002-2004), I.D. Petsalakis (P.I.), G. Theodorakopoulos
5. Development of a theoretical method for the study of interactions between open shell molecular units. Applications to moieties containing transition metals, GSRT (Greece-Poland), (2001-2002), I.D. Petsalakis (P.I.), G. Theodorakopoulos
6. Theoretical study of the spectroscopy of polyatomic alkaline earth containing molecules, GSRT (Greece-Poland), (2001-2002), G. Theodorakopoulos (P.I.), I.D. Petsalakis
7. New photo resistive self-organized materials for nanolithography in the ultraviolet, GSRT / EPET-II / PENED '99, (2000-2001), A.C. Cefalas (PI), I.D. Petsalakis, E. Sarantopoulou, Z. Kollia
8. Three-vector correlations in gas-phase chemistry, GSRT (Greece-Russia), (1999-2000), I.D. Petsalakis (P.I.), G. Theodorakopoulos

DISTINCTIONS

- Lady Davis visiting professor in the faculty of science at the Hebrew University of Jerusalem 15/9/2013-31/12/2013
- Scholarship from EC (Marie Curie Individual Fellowship) 1/11/1999-31/10/2000
- Marie Curie Fellow since 1999
- Scholarship from the Alexander Von Humboldt Foundation from 1/11/1995-31/10/1996
- Alexander von Humboldt Fellow since 1995
- Scholarship from the Theoretical and Physical Chemistry Institute of the National Hellenic Research Foundation 1/8/1980-28/2/1986

PUBLICATION: 179 refereed articles in international scientific journals with 2310 citations, h-index 24 (ISI web of science 21 Sept. 2021)

SELECTED PUBLICATIONS

- (Tzeli, D.; Petsalakis, I. D.; Theodorakopoulos, G.; Rahman, F.-U.; Yu, Y.; Rebek Jr., J. The Role of Electric Field, Peripheral Chains, and Magnetic Effects on Significant H-1 Up field Shifts of the Encapsulated Molecules in Chalcogen-Bonded Capsules. *Phys. Chem. Chem. Phys.* 2021, 23 (35), 19647–19658. <https://doi.org/10.1039/d1cp02277f>.
- (Rahman, F.-U.; Tzeli, D.; Petsalakis, I. D.; Theodorakopoulos, G.; Ballester, P.; Rebek Jr., J.; Yu, Y. Chalcogen Bonding and Hydrophobic Effects Force Molecules into Small Spaces. *J. Am. Chem. Soc.* 2020, 142 (12), 5876–5883. <https://doi.org/10.1021/jacs.0c01290>.
- (Tzeli, D.; Petsalakis, I. D. Physical Insights into Molecular Sensors, Molecular Logic Gates, and Photosensitizers in Photodynamic Therapy. *J. Chem.* 2019, 2019. <https://doi.org/10.1155/2019/6793490>.
- (Ghosh, K.; Tarafdar, D.; Petsalakis, I. D.; Theodorakopoulos, G. A Pyridinium-Urea-Coupled Polyether Receptor for the Selective Sensing of Lysine and Cell Imaging. *European J. Org. Chem.* 2017, 2017 (2), 355–362. <https://doi.org/10.1002/ejoc.201601203>.
- (Lathiotakis, N. N.; Theodorakopoulos, G.; Petsalakis, I. D. Electron Transfer through Organic Molecular Wires: A Theoretical Study. *Chem. Phys. Lett.* 2017, 667. <https://doi.org/10.1016/j.cplett.2016.11.044>.
- (Tzeli, D.; Mercouris, T.; Theodorakopoulos, G.; Petsalakis, I. D. Time-Evolution Study of Photoinduced Charge-Transfer in Tertiary Amine-Fluorophore Systems. *Comput. Theor. Chem.* 2017, 1115, 197–207. <https://doi.org/10.1016/j.comptc.2017.06.019>.
- (Petsalakis, I. D.; Theodorakopoulos, G.; Buchman, O.; Baer, R. Applicability of Mulliken's Formula for Photoinduced and Intramolecular Charge-Transfer Energies. *Chem. Phys. Lett.* 2015, 625, 98–103. <https://doi.org/10.1016/j.cplett.2015.02.040>.
- (Petsalakis, I. D.; Theodorakopoulos, G. Boronic Acid Sensors for Saccharides: A Theoretical Study. *Chem. Phys. Lett.* 2013, 586, 111–115. <https://doi.org/10.1016/j.cplett.2013.09.025>.
- (Petsalakis, I. D.; Theodorakopoulos, G. Molecular Orbital Assistance in the Design of Intramolecular and Photoinduced Electron Transfer Systems. *Chem. Phys. Lett.* 2012, 525–26, 105–109. <https://doi.org/10.1016/j.cplett.2012.01.002>.
- (Tzeli, D.; Theodorakopoulos, G.; Petsalakis, I. D.; Ajami, D.; Rebek Jr., J. Conformations and Fluorescence of Encapsulated Stilbene. *J. Am. Chem. Soc.* 2012, 134 (9), 4346–4354. <https://doi.org/10.1021/ja211164b>.
- (Irimia, D.; Petsalakis, I. D.; Theodorakopoulos, G.; Janssen, M. H. M. Coherent Oscillatory Femtosecond Dynamics in Multichannel Photodynamics of NO₂ Studied by

- Spatially Masked Electron Imaging. *J. Phys. Chem. A* 2010, 114 (9), 3157–3166. <https://doi.org/10.1021/jp909031p>.
- (Ghosh, K.; Masanta, G.; Froehlich, R.; Petsalakis, I. D.; Theodorakopoulos, G. Triphenylamine-Based Receptors in Selective Recognition of Dicarboxylic Acids. *J. Phys. Chem. B* 2009, 113 (22), 7800–7809. <https://doi.org/10.1021/jp901151w>.
 - (Petsalakis, I. D.; Kerkines, I. S. K.; Lathiotakis, N. N.; Theodorakopoulos, G. Emitting and Electron-Transfer Electronic States of Tertiary Amine-Fluorophore Sensor Systems. *Chem. Phys. Lett.* 2009, 474 (4–6), 278–284. <https://doi.org/10.1016/j.cplett.2009.04.080>.
 - (Petsalakis, I. D.; Tagmatarchis, N.; Theodorakopoulos, G. Theoretical Study of Fulleropyrrolidines by Density Functional and Time-Dependent Density Functional Theory. *J. Phys. Chem. C* 2007, 111 (38), 14139–14149. <https://doi.org/10.1021/jp0743774>.
 - (Harikumar, K. R.; Petsalakis, I. D.; Polanyi, J. C.; Theodorakopoulos, G. Parent- and Daughter-Mediated Halogenation Reactions Modeled for 1,2- and 1,4-Dibromobenzene at Si(111)-7x7. *Surf. Sci.* 2004, 572 (2–3), 162–178. <https://doi.org/10.1016/j.susc.2004.08.042>.
 - (Luque, J.; Hudson, E. A.; Booth, J. P.; Petsalakis, I. D. Broadband Absorption and Ab Initio Results on the CF C-2 Sigma(+)-X-2 Pi System. *J. Chem. Phys.* 2003, 118 (3), 1206–1213. <https://doi.org/10.1063/1.1526637>.
 - (Petsalakis, I. D.; Polanyi, J. C.; Theodorakopoulos, G. Theoretical Study of the Induced Attachment of Benzene to Si(111) 7 x 7. *Surf. Sci.* 2003, 544 (2–3), 162–169. <https://doi.org/10.1016/j.susc.2003.07.003>.
 - (Petsalakis, I. D.; Theodorakopoulos, G.; Child, M. S. The Rydberg States of NO₂: Vibrational Autoionization of the Nd Sigma States. *J. Chem. Phys.* 2001, 115 (22), 10394–10403. <https://doi.org/10.1063/1.1415084>.
 - (Honigmann, M.; Hirsch, G.; Buenker, R. J.; Petsalakis, I. D.; Theodorakopoulos, G. Complex Coordinate Calculations on Autoionizing States of HeH and H-2. *Chem. Phys. Lett.* 1999, 305 (5–6), 465–473. [https://doi.org/10.1016/S0009-2614\(99\)00408-X](https://doi.org/10.1016/S0009-2614(99)00408-X).
 - (Petsalakis, I. D. Theoretical Study on Electronic States of Carbon Monofluoride and on the Predissociation of the Lower Lying States. *J. Chem. Phys.* 1999, 110 (22), 10730–10737. <https://doi.org/10.1063/1.478997>.
 - (Petsalakis, I. D.; Theodorakopoulos, G.; Child, M. S. Ab Initio Multichannel Quantum Defects for the (1)A(1) Rydberg States of H₂O. *J. Phys. B-ATOMIC Mol. Opt. Phys.* 1995, 28 (24), 5179–5192. <https://doi.org/10.1088/0953-4075/28/24/004>.
 - (Mercouris, T.; Petsalakis, I. D.; Nicolaides, C. A. Time-Dependent Laser-Induced Molecular Formation From Repulsive Surfaces. *Chem. Phys. Lett.* 1993, 208 (3–4), 197–203. [https://doi.org/10.1016/0009-2614\(93\)89061-L](https://doi.org/10.1016/0009-2614(93)89061-L).

- Petsalakis, I. D.; Theodorakopoulos, G.; Nicolaides, C. A.; Buenker, R. J. Nearly Diabatic States by Maximization of the Non-Orthogonal Overlap Between Model-Diabatic and MRD-CI Wave-Functions. *Chem. Phys. Lett.* 1991, 185 (3–4), 359–364. [https://doi.org/10.1016/S0009-2614\(91\)85075-8](https://doi.org/10.1016/S0009-2614(91)85075-8).
- (Petsalakis, I. D.; Metropoulos, A.; Theodorakopoulos, G.; Nicolaides, C. A. An Estimate of the Lifetime of Excited Tetrahydrogen. *Chem. Phys. Lett.* 1989, 158 (3–4), 229–232. [https://doi.org/10.1016/0009-2614\(89\)87326-9](https://doi.org/10.1016/0009-2614(89)87326-9).
- Petsalakis, I. D.; Theodorakopoulos, G.; Nicolaides, C. A.; Buenker, R. J.; Peyerimhoff, S. D. Nonorthogonal CI for Molecular Excited-States. 1. The Sudden Polarization Effect in 90-Degrees Twisted Ethylene. *J. Chem. Phys.* 1984, 81 (7), 3161–3167. <https://doi.org/10.1063/1.448020>.

[List of publications](#)