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EDUCATION

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

Ph.D. in Molecular Physics, Capodistrian 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 NC 27695-8204 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 St. 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 –

Gausstrasse 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

- (i) Member of team (I.D. Petsalakis, G. Theodorakopoulos and N. Tagmatarchis-coordinator) involved in NANOHOST project (FP7-REGPOT-2007-1) Feb. 1,2008-Feb.,2011
- (ii) FP7-PEOPLE- IRG-2008, 2008-2012
- (iii) Greece-Slovakia joint research and technology project, 2005-2007.
- (iv) MCIF-EU, 2003-2004, EU MCIF (2000-2001)
- (v) NATO PST/CLG.977379, (2009-2012), NATO PST/CLG.978504 , (2002-2003), NATO - CRG (2001-2002), NATO - CRG (1998-2000),
- (vi) 2 X, Greece-Poland joint research and technology project 2001-2003,
- (vii) Greece-Russia joint research and technology project 1999-2000,
- (viii) INTAS 1999, 2000-2003,. (ix) GSRT-PRAXE-17 (2002-2004)
- (x) Participation in other NATO and GSRT bilateral projects.

PARTICIPATION IN INTERNATIONAL MEETINGS

I have participated in 20 international conferences and two local, in Greece, I have been co-organizer in two conferences, and I have given many invited talks in Greek, German, Israel and Canadian universities.

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) from 1/11/1999-31/10/2000.
- Marie Curie Fellow
- Scholarship from the Alexander Von Humboldt Foundation from 1/11/1995-31/10/1996
- Alexander von Humboldt Fellow

- Scholarship from the Theoretical and Physical Chemistry Institute of the National Hellenic Research Foundation from 1/8/1980-28/2/1986

PUBLICATIONS: 152 refereed articles in international scientific journals and 1743 citations (ISI web of science Feb.2017)

SELECTED PUBLICATIONS

- N. N. Lathiotakis, G. Theodorakopoulos and I. D. Petsalakis 'Electron transfer through organic molecular wires: A theoretical study' [Chem.Phys.Let.,667, 45-50 \(2017\)](#)
- D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, 'Molecular logic gates based on benzo-18-crown-6 ether of styrylquinoline: a theoretical study' [PCCP 18, 32132-32145, \(2016\)](#)
- I. D. Petsalakis, G. Theodorakopoulos, O. Buchman, R. Baer, "Applicability of Mulliken's formula for photoinduced and intramolecular charge-transfer energies", [Chem. Phys. Let. 625, 98-103, \(2015\)](#)
- B.Pappas, I.D.Petsalakis, G.Theodorakopoulos and J.Whitten "CI and DFT Studies of the Adsorption of the Nerve Agent Sarin on Surfaces" [J. Phys. Chem. C, 23042 \(2014\)](#)
- M. G. Sarwar, D. Ajami, G. Theodorakopoulos, I. D. Petsalakis, and J. Rebek, Jr, "Amplified Halogen Bonding in a Small Space", [J. Amer.Chem.Soc. communication 135,13672 \(2013\)](#)
- I. D. Petsalakis and G. Theodorakopoulos, Boronic Acid sensors for saccharides: A theoretical study [Chem. Phys.Let. 586, 1-115 \(2013\)](#)
- D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr,"Conformations and fluorescence of encapsulated stilbene" [J. Amer. Chem.Soc.134, 4346 \(2012\)](#)
- I.D.Petsalakis and G.Theodorakopoulos, " Molecular orbital assistance in the design of intramolecular and photoinduced electron transfer systems",[Chem. Phys.Lett., 525,105-109 \(2012\)](#)
- D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr, "Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes" [J. Amer. Chem.Soc. 16977, 133 \(2011\)](#)
- I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and J. Rebek, Jr, "Excited state intramolecular proton transfer in hydroxy oxime-based chemical sensors" [The J. Phys. Chem. A. 115, 834 \(2011\)](#)

- I. D. Petsalakis and G. Theodorakopoulos "Theoretical calculations on the potential energy curves of electronic states of CF. Rydberg states of CF above the lowest ionization limit" [Chem.Phys.Lett. 508, 17 \(2011\)](#)
- I.D. Petsalakis, I.S.K. Kerkines, N.N. Lathiotakis and G. Theodorakopoulos "Emitting and electron transfer electronic states of tertiary amine-fluorophore sensor systems" , [Chem. Phys. Lett. 474, 278 \(2009\)](#)
- K. R. Harikumar, I. D. Petsalakis, J. C. Polanyi, and G. Theodorakopoulos, Theoretical study of the halogenation reactions of 1,2- and 1,4-dibromobenzene at Si(111)-7×7, [Surface Science 572, 162 \(2004\)](#)
- I.D. Petsalakis G.Theodorakopoulos, Yan 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 \(1998\)](#)

List of publications:

http://www.eie.gr/nhrf/institutes/tpci/cvs/cv-petsalakis_list.pdf