

IOANNIS D. PETSALAKIS**AFFILIATION**

Director of Research. Theoretical and Physical Chemistry Institute, The National Hellenic Research Foundation, 48 Vas. Constantinou Ave., Athens 116 35, Greece, Tel:+30-7273-807, Fax:+30-7273-794, email: idpet@eie.gr

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** 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

(b) Bergische Universität – Gesamthochschule **Wuppertal**, Theoretische Chemie,Fachbereich 9 – Gausstrasse 20, D-42097 Wuppertal, Germany

From October 1982 – present, 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.

(c) **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.

(d) **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 developments of theoretical methods and applications have been carried out. The theoretical methods are within the framework of Quantum Mechanics and are devoted to

- (a) the calculation of “difficult” electronic states involving near degeneracies and symmetry breaking (Non-orthonormal configuration interaction, Multi-Reference single and Double excitations Configuration Interaction)
- (b) the calculation of predissociation resonances (Complex coordinate rotation)
- (c) time-dependent studies of photodissociation as well as laser-induced molecular formation,
- (d) the prediction of the spectra of diatomic and triatomic molecules,
- (e) the prediction of highly excited molecular states (Multi-channel Quantum Defect Theory)
- (f) calculations including relativistic effects for molecules with heavy atoms
- (g) theoretical investigation of attachment of molecules on Si(111) surface.
- (h) Theoretical studies in donor-acceptor carbon based materials

EXTERNAL FUNDING PROJECTS

Participant or coordinator in EU/MCIF, NATO, Alexander von Humboldt and GERT/PENED’99 projects.

PARTICIPATION IN INTERNATIONAL MEETINGS

I have participated in 17 international and two local, in Greece, conferences and I have given many invited talks in Greek, German and Canadian universities.

DISTINCTIONS

- Scholarship from the Theoretical and Physical Chemistry Institute of the National Hellenic Research Foundation from 1/8/1980-28/2/1986
- Scholarship from the Alexander Von Humboldt Foundation from 1/11/1995-31/10/1996
- Alexander von Humboldt Fellow
- Scholarship from EC (Marie Curie Individual Fellowship) from 1/11/1999.
- Marie Curie Fellow