

## CURRICULUM VITAE

Stavros C. Farantos

Department of Chemistry, University of Crete, and  
Institute of Electronic Structure and Laser,  
Foundation for Research and Technology-Hellas,  
Iraklion, Crete 711 10, Greece

- Born** : June 3rd, 1951, Piraeus.
- October 1969 - June 1973** : First degree in Chemistry,  
Department of Chemistry, University of Athens.
- October 1973 - February 1976** : Military service.
- April 1976 - September 1978** : Ph. D. degree in Theoretical Chemistry,  
University of Sussex (Title :  
Potential Energy Surfaces and Molecular  
Dynamics of Chlorine - Oxygen system  
Supervisor: Professor John N. Murrell (FRS).
- October 1978 - October 1981** : Research Fellow, School of  
Molecular Sciences, University of Sussex.
- November 1981-September 1984** : Research Scientist, Theoretical and  
Physical Chemistry Institute, National  
Hellenic Research Foundation.
- October 1984 - July 1989** : Assistant Professor in Chemistry,  
University of Crete, and Research  
Scientist in the IESL, Foundation for  
Research and Technology-Hellas.
- July 1987 - September 1987** : Visiting Researcher, Department of  
Chemistry, University of Bielefeld, Germany.
- July 1989 - June 1990** : Visiting Professor, Departments of  
Chemistry and Physics, University of  
Southern California, California, USA.
- August 1989 - March 1994** : Associate Professor in Chemistry,  
University of Crete, and Research  
Scientist in IESL, Foundation for  
Research and Technology-Hellas.
- April 1994 - Present** : Professor in Chemistry,  
University of Crete, and Research  
Scientist in IESL, Foundation for  
Research and Technology-Hellas.
- September 1995 - December 1995  
and following years** : Visiting Professor,  
Max Planck Institute fur Dynamic und Selbstorganisation,  
Goettingen, Germany.
- July 1996 and March 1999** : Visiting Professor, Pacific Northwest National  
Laboratory Battell, Richland, Washington State.
- September 2005** : Visiting Professor, Dept. of Chemistry,  
Univ. of New Mexico, Albuquerque, USA.  
Albuquerque, USA.
- June 2007** : Visiting Professor, Groupe de Spectroscopie  
Moleculaire et Atmospherique, Faculte de  
Sciences, Universite de Reims, Reims, France.

### OTHER ACTIVITIES

- [1] Member of the NATO Collaborative Research Grants Advisory Panel, 1995 - 1998.
- [2] Member of the NATO Physical and Engineering Science and Technology Advisory Panel, 1999.
- [3] Director of the Computer Center of University of Crete and FORTH, April 1996 - April 1997.
- [4] FORTH representative in CECAM (Centre Europeen de Calcul Atomique et Moleculaire).
- [5] Member of the Scientific Advisory Committee, of the Institute of Theoretical and Physical Chemistry (ITPC), National Hellenic Research Foundation (NHRF)
- [6] Associate director of the Institute of Electronic Structure and Laser (2004-)
- [7] FORTH representative in European Science Foundation PESC-Physics and Engineering Science Council (2005-)

### RESEARCH INTERESTS

- [1] Spectroscopy, dynamics and thermodynamics of atomic and molecular clusters. **Ref. [51,69].**
- [2] Theoretical vibrational spectroscopy of small polyatomic molecules with atmospheric interest. **Ref. [96].**
- [3] Elementary chemical reactions - isomerization, dissociation - in small polyatomic molecules. Applications of nonlinear mechanics. **Ref. [80,95,104,118].**
- [4] Energy localization and redistribution in biological molecules. **Ref. [108,111,116,121].**
- [5] Development of methods and computer codes for novel high performance computational schemes - grid computing - for classical and quantum dynamics. **Ref. [70,81,85,120].**

### GRANTS 2000-2010

- [16] **European Network for Advanced Computing Technology for Science** (ENACTS), with the EPCC, 2000-2004. ENACTS 47604 Euro.
- [17] **IKYDA 2000**, Greek-German Program, Quantum mechanical studies of Si-Ge and Si-C clusters with Prof. Sigrid Peyerimhoff, Institute of Physical and Theoretical Chemistry, Univ. of Bonn, 2000-2003, 18000 Euro.
- [18] **Applied Molecular Spectroscopy**: a postgraduate program, with the Department of Chemistry of Univ. of Athens, the Department of Chemical Engineering of Univ. of Patras, ITPC-NHRF, and IESL-FORTH, 2001-2003. EPEAEK-II 240000 Euro.
- [19] **Hrakteitos**: PhD scholarship, Ministry of Education, Study of elementary chemical reactions of biological molecules with nonlinear mechanics methods, 2003-2005, 33000 Euros.
- [20] **Pythagoras**: Postdoctoral scholarship, Ministry of Education, New structures for hydrogen storage in carbon nanotubes. 2004-2006, 80000 Euros.
- [21] **Pythagoras II**: Research Support, Ministry of Education, Dynamics and reactivity in protein reactions: spectroscopy and theoretical studies. 2005-2006, 50000 Euros.
- [22] **ToK-DEV**: Grid Computational Chemistry (GRID-COMP-CHEM), 2006-2010, 720842 Euros.

### PUBLICATIONS

Articles in International Journals and Books : [121]  
Special Articles : [3]  
Books in English : [1]  
Books Translated in Greek : [2]  
Conferences-Presentations and Invited Talks : [64]

PhD Thesis : [6]

Ms Thesis : [4]

### REPRESENTATIVE PUBLICATIONS

- [51] A. Vegiri, and S. C. Farantos. *Classical Dynamics of Hydrogen Bonded Systems: Water Clusters*. **J. Chem. Phys.**, 98(5):4059–4075, 1993.
- [69] S. S. Xantheas, G. S. Fanourgakis, S. C. Farantos and M. Velegrakis. *Spectroscopic Constants of the  $X^2\Sigma^+$  and  $A^2\Pi$  States of  $Sr^+Ar$  from First Principles: Comparison with experiment*. **J. Chem. Phys.**, 108:46, 1998.
- [70] S. C. Farantos. *POMULT: A Program for Computing Periodic Orbits in Hamiltonian Systems Based on Multiple Shooting Algorithms*. **Comp. Phys. Comm.**, 108:240, 1998.
- [80] H. Ishikawa, R. W. Field, S. C. Farantos, M. Joyeux, J. Koput, C. Beck and R. Schinke. *HCP - CPH Isomerization: Caught in the Act*, volume 50. **Annual Review of Physical Chemistry**, 1999.
- [81] R. Guantes and S. C. Farantos. *High Order Finite Difference Algorithms for Solving the Schrödinger Equation in Molecular Dynamics*. **J. Chem. Phys.**, 111:10827, 1999.
- [85] S. Stamatiadis, R. Prosmiiti, and S. C. Farantos. *AUTO\_DERIV: Tool for automatic differentiation of a FORTRAN code*. **Comp. Phys. Comm.**, 127:343–355, 2000.
- [95] M. Joyeux, S. C. Farantos and R. Schinke. *Highly Excited Motion in Molecules: Saddle-Node Bifurcations and their Fingerprints in Vibrational Spectra*. **J. Phys. Chem.**, (feature article): 5407–5421, 2002.
- [96] Rudiger Siebert, Paul Fleurat-Lessard, R. Schinke, Martina Bittererova, and S. C. Farantos. *The Vibrational Spectrum of Ozone up to Dissociation Threshold: Dynamics calculations on an accurate potential energy surface*. **J. Chem. Phys.**, 116(22):9749–9767, 2002.
- [104] M. Joyeux, S. Yu. Grebenshchikov, J. Bredenbeck, R. Schinke, and S. C. Farantos. *Intramolecular Dynamics Along Isomerization and Dissociation Pathways, in "Geometrical Structures of Phase Space in Multi-Dimensional Chaos"*. **Advances in Chemical Physics**, 130:267–303, 2005.
- [108] Andreas Mavrandonakis, Stavros C. Farantos, and George E. Froudakis. *Glycine Interaction with Carbon Nanotubes: An ab Initio Study*. **J. Phys. Chem. B**, 110:6048–6050, 2006.
- [111] S. C. Farantos. *Periodic Orbits in Biological Molecules: Phase Space Structures and Selectivity in Alanine Dipeptide*. **J. Chem. Phys.**, 126(17):175101–175107, 2007.
- [116] Vangelis Daskalakis, Stavros C. Farantos, and Constantinos Varotsis. *Assigning vibrational spectra of ferryl-oxo intermediates of Cytochrome c Oxidase by periodic orbits and Molecular Dynamics*. **J. Am. Chem. Soc.**, 130(37):12385–12393, 2008.
- [118] Stavros C. Farantos, Reinhard Schinke, Hua Guo, and Marc Joyeux. *Energy Localization in Molecules, Bifurcation Phenomena, and their Spectroscopic Signatures: The Global View*. **Chemical Reviews**, in press, 2009.
- [120] Jaime Suarez, Stavros C. Farantos, Stamatis Stamatiadis, and Lucas Lathouwers. *A method for solving the molecular Schroedinger Equation in Cartesian coordinates via angular momentum projection operators*. **Comp. Phys. Comm.**, doi:10.1016/j.cpc.2009.06.004, 2009.
- [121] Massimiliano Porrini, Vangelis Daskalakis, S. C. Farantos, and Constantinos Varotsis. *Heme Cavity Dynamics of Photodissociated CO from ba3-Cytochrome c Oxidase: the Role of Ring-D Propionate*. **J. Phys. Chem. B**, in press, 2009.