# 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

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| **Born** | : June 3rd, 1951, Piraeus. |
| **Father of twin sons** | : Constantine and Plato |
| **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 systems, 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. |

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| **July 1989 - June 1990** | : Visiting Scholar, 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** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **July 1996** | : Visiting Professor, Pacific Northwest National Laboratory, Battell, Richland, Washington State. |
| **September 1997** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **November 1998** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **March 1999** | : Visiting Professor, Pacific Northwest National Laboratory, Battell, Richland, Washington State, USA. |
| **Octomber-November 2000** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **December 2001** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **January 2003** | : Visiting Professor, Max Planck Institute für Physik Komplexer Systeme, Dresden, Germany. |

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| **July 2003** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **January 2004** | : Visiting Professor, Max Planck Institute für Strömungsforschung, Göttingen, Germany. |
| **September 2005** | : Visiting Professor, Dept. of Chemistry Univ. of New Mexico, Albuquerque, USA. |
| **June 2006** | : Visiting Professor, Max Planck Institut für Dynamik und Selbstorganisation, Göttingen, Germany. |
| **June 2007** | : Visiting Professor, Groupe de Spectroscopie Moleculaire et Atmospherique, Faculte des Sciences, Universite de Reims, Reims, France. |
| **January-May 2010** | : Visiting Professor, Department of Chemistry University of Perugia, Italy. |
| **June 2011** | : Visiting Professor, Max Planck Institut für Dynamik und Selbstorganisation, Göttingen, Germany. |
| **September 2012** | : ERASMUS Lectures Department of Physical Chemistry, University of Barcelona, Barcelona, Spain. |
| **November 25-December 10 2012** | : Visiting Professor, Max Planck Institut für Dynamik und Selbstorganisation, Göttingen, Germany. |

## RESEARCH INTERESTS

[1] Theoretical vibrational spectroscopy of small polyatomic molecules with atmospheric interest.

[2] Elementary chemical reactions - isomerization, dissociation - in small polyatomic molecules.

[3] Energy localization and redistribution in biological molecules.

[4] Spectroscopy, dynamics and thermodynamics of atomic and molecular clusters.

[5] Development of methods and computer codes for novel high performance, high throughput computational schemes - Grid & Cloud computing - for classical and quantum dynamics.

## 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] Pacific Northwest National Laboratory Affiliate Staff Scientist (PASS), since July 1995.

[6] Member of the organizing committee of the NATO-ASI, "Recent Theoretical and Experimental Advances in Hydrogen-Bonding Clusters", Elounda, Crete, Greece, June-22 - July 4, 1997.

[7] Member of the organizing committee of the CECAM workshop, "Spectroscopy and Computational Challenges in Vibrationally Highly Excited Polyatomic Molecules", Lyon, France, July 10-12, 2000.

[8] Member of the Scientific Advisory Committee, of the Institute of Theoretical and Physical Chemistry (ITPC), National Hellenic Research Foundation (NHRF)

[9] Member of the organizing committee of the CECAM-SIMU workshop, "Quantum Dynamics of Condensed Phase Systems", Rethymnon, Crete, June 24-28, 2002.

[10] Greece representative in Management Committee of COST D23 - METACHEM (Metalaboratories for Complex Computational Applications in Chemistry),

2000 - 2005

[11] Scientific director of the postgraduate program "Applied Molecular Spectroscopy",
Department of Chemistry, University of Crete,
1998 - present

[12] Member of the organizing committee of the CECAM workshop,
"ENERGY LOCALIZATION: From Small Polyatomic Molecules to Large Biomolecules",
Lyon, France, September 6-8, 2004.
with Sergej Flach, Max Planck Institute for the Physics of Complex Systems
Noethnitzer Strasse 38, 01187 Dresden, GERMANY, and
Michel Peyrard, Laboratoire de Physique, Ecole Normale Superieure de Lyon,
46, Allee d'Italie, 69364 Lyon CEDEX 07 - FRANCE

[13] Deputy director of the Institute of Electronic Structure and Laser (2004-2010)

[14] FORTH representative in European Science Foundation
PESC - Physics and Engineering Science Council (2005-2011),

## PUBLICATIONS

### PhD Thesis

*Potential Energy Surfaces and Molecular Dynamics of Chlorine-Oxygen systems*,
Supervisor, Prof. John N. Murrell (FRS), Department of Chemistry, University of Sussex, 1978.

### Articles in International Journals and in Books after invitation

[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20] [21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38] [39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58] [59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78] [79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97] [98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116] [117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132]

### Other Articles

[133, 134, 135, 136, 137]

### Books in English

[138]

**Books Translated in Greek**

[139, 140]

## ADDRESS


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|---|---|
| **Name** | : Prof. Stavros C. Farantos |
| | : |
| **Address** | : Institute of Electronic Structure and Laser |
| | : Foundation for Research and Technology-Hellas, and |
| | : Department of Chemistry, University of Crete |
| | : P.O. BOX 1527 |
| | : Iraklion 711 10, Crete |
| | : Greece |
| | : |
| **Telephone** | : +30-2810-39 1813 (Personal) |
| | : +30-2810-39 1301-3 (Secretaries) |
| | : +30-2810-54 5061 (Chemistry) |
| **FAX** | : +30-2810-39 1305 |
| **E-Mail** | : farantos@iesl.forth.gr |
| **URL** | : http://TCCC.iesl.forth.gr/ |

# References


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Analytical Potentials for Triatomic Molecules from Spectroscopic Data: III. Application to $A_2B$ molecules whose surfaces have more than one minimum.
*Mol. Phys.*, 34(4):947–962, 1977. 5

[2] J. N. Murrell, and **S. Farantos**.
An Analytical Function for the Potential Energy Surface of Ozone.
*Mol. Phys.*, 34(4):1185–1188, 1977. 5

[3] **S. C. Farantos,** and J. N. Murrell.
Classical Dynamics of the $O + ClO \rightarrow Cl + O_2$ and $Cl + O_3 \rightarrow ClO + O_2$ Reactions.
*Int. J. Quantum Chem.*, 14(5):659–674, 1978. 5

[4] **S. C. Farantos,** and J. N. Murrell.
A Classical Trajectory Study of the Reaction $H + HCO \rightarrow H_2 + CO$.
*Mol. Phys.*, 40(4):883–891, 1980. 5

[5] **S. C. Farantos,** and J. N. Murrell.
Application of the Strong Coupling-Correspondence Principle to Atom - Triatom Collinear Collisions.
*Int. J. Quantum Chem.*, 19:95–104, 1981. 5

[6] **S. C. Farantos,** and J. N. Murrell.
On the Transition from Quasiperiodic to Stochastic Classical Motion on Real Polyatomic Potential Energy Surfaces.
*Chem. Phys.*, 55:205–214, 1981. 5

[7] **S. C. Farantos,** and J. N. Murrell.
Studies on Atom - Triatom Scattering: Classical Dynamics of $H + C_2H$ Collisions.
*J. Chem. Soc. Faraday Trans. II*, 77:2279–2288, 1981. 5

[8] **S. C. Farantos,** J. N. Murrell, and J. C. Hijduk.
Monte Carlo Calculations of Classical Density of States for Non-Separable Polyatomic Potential Energy Surfaces.
*Chem. Phys.*, 68:109–117, 1982. 5

[9] **S. C. Farantos**.
Evaluation of an Upper Bound of the Maximal Lyapunov Characteristic Number by Monte Carlo Integration in the Chaotic Regions of Phase Space.
*Chem. Phys.*, 71:157–160, 1982. 5

[10] **S. C. Farantos**.
Exponentially Divergent Trajectories and RRKM Behaviour of $Ar_3$ Clusters.
*Chem. Phys. Letters*, 92:379–382, 1982. 5

[11] J. N. Murrell, W. Craven, and **S. C. Farantos**.
Classical Dynamics of the Reaction $S(^3P) + O_2(^3\Sigma_g^-)$.
*Mol. Phys.*, 49(5):1077–1084, 1983. 5

[12] **S. C. Farantos,** G. Theodorakopoulos, and C. A. Nicolaides.
A Non-van der Waals Minimum on the $He(^1S) + H_2(B^1\Sigma_u^+)$ Excited Surface.
*Chem. Phys. Letters*, 100:263–267, 1983. 5

[13] **S. C. Farantos**.
Studies on the Statistical Behaviour of $Ar$ Clusters: The $Ar_4$ Case.
*J. Phys. Chem.*, 87:5061–5064, 1983. 5

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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*, 17:1453–1462, 1984. 5

[15] **S. C. Farantos,** J. N. Murrell, and S. Carter.
Analytical Ab Initio Potential Energy Surfaces for the Ground and the First Singlet Excited States of $HeH_2$.
*Chem. Phys. Letters*, 108:367–372, 1984. 5

[16] J. Tennyson, and **S. C. Farantos**.
Vibrational Chaos in $KCN$: A Comparison of Quantum and Classical Calculations.
*Chem. Phys. Letters*, 109:160–165, 1984. 5

[17] **S. C. Farantos**.
A Quasiclassical Study of Collisions of $He$ with $HD(B^1\Sigma_u^+)$.
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Ro - Vibrational Spectrum of the Excited Potential Energy Surface of $He + H_2(B^1\Sigma_u^+)$.
*J. Chem. Phys.*, 82(4):2163–2164, 1985. 5

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*J. Chem. Phys.*, 82(2):800–809, 1985. 5

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*Chem. Phys.*, 93(2):237–244, 1985. 5

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On the Vibrational Born-Oppenheimer Separation Scheme for Molecules with Regular and Chaotic States.
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A Classical Trajectory Study of the Reaction $He(^1S) + H_2(B^1\Sigma_u^+) \rightarrow HeH(A^2\Sigma^+) + H(^2S)$.
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Ab Initio Potential Energy Surfaces for Studying the Quenching of $CH(A^2\Delta)$ by $H_2(X^1\Sigma_g^+)$.
*Chem. Phys. Letters*, 167(4):278–284, 1990. 5

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Classical Mechanical Methods for Extracting the Dynamics from Stimulated-Emission Pumping Spectra.
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The Extraction of Dynamics and the Classical Mechanical Simulation of Low Resolution Regular and Chaotic Spectra: $HCN/HNC$.
*J. Chem. Phys.*, 93(1):76–86, 1990. 5

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Classical Dynamical Analysis of the Vibrational Spectra for Small Polyatomic Molecules.
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The Photodissociation of $O_3$: A Classical Dynamical Approach for the Interpretation of the Recurrences in the Autocorrelation Function.
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On the Consistency Between Recent Experimental Results and a Previous Theoretical Analysis of $HCN/HNC$.
*J. Chem. Phys.*, 94(1):2376, 1991. 5

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Periodic Orbits and Quantum Localization in the van der Waals System $CO - Ar$.
*Chem. Phys.*, 154:55–62, 1991. 5

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The Importance of Periodic Orbits in Analysing Photodissociation Resonances: the $O_3$ Case.
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Spectroscopy and Dynamics of Vibrationally Excited Molecules: A Phase Space Structure Analysis. In T. Bountis, editor, *Chaotic Dynamics: Theory and Practice*, pages 301–316. Plenum Co. Ltd., 1992. 5

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Classical Dynamics of Hydrogen Bonded Systems: Water Clusters.
*J. Chem. Phys.*, 98(5):4059–4075, 1993. 5

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Periodic Orbits as a Probe to Reveal Exotic States: The Saddle-Node States.
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Testing Molecular Potential Functions with Bifurcation Diagrams of Periodic Orbits .
*Mol. Phys.*, 80(6):1499–1505, 1993. 5

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Minimum Structures and Dynamics of Small Water Clusters.
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Water Clusters: The $(H_2O)_{64}$ case.
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Complex Unstable Periodic Orbits and their Manifestation in Classical and Quantum Dynamics.
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Methods for Locating Periodic Orbits in Highly Unstable Systems.
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Periodic Orbits, Bifurcation Diagrams and the Spectroscopy of $C_2H_2$ System.
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A Periodic Orbit Analysis of the Vibrationally Highly Excited LiNC/LiCN:
a comparison with quantum mechanics.
*J. Chem. Phys.*, 104(8):2921–2931, 1996. 5

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Potential Functions and Static and Dynamic Properties of $Mg^{m+}Ar_n, m = 1, 2;\ n = 1 - 18$ clusters.
*J. Phys. Chem.*, 100:3900–3909, 1996. 5

[63] **S. C. Farantos**.
Exploring Molecular Vibrations with Periodic Orbits.
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Normal Mode and Isomerization Bending States in HCP:
Periodic Orbit Assignment and Spectroscopic Signature.
*J. Chem. Phys. (Communication)*, 104(24):10055–10058, 1996. 5

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*J. Comput. Chem.*, 18:1011–1022, 1997. 5

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An Effective Transition State for a Complex Cluster Isomerization Process: comparison between anharmonic and harmonic models for $Mg^+Ar_{12}$.
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*Chem. Phys. Letters*, 277:456–464, 1997. 5

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by **S. C. Farantos**$^*$.

[52] International Conference of Computational Methods in Sciences
and Engineering 2005 (ICCMSE 2005)
HOTEL POSIDON, Loutraki, Greece, 21-26 October, 2005.
Grid Enabled Molecular Dynamics: classical and quantum algorithm
by **S. C. Farantos**$^*$, S. Stamatiadis, L. Lathouwers and R. Guantes.

[53] Theoretical Chemistry and Computational Modelling (TCCM)
Perugia, Italy, 18 July-13 August, 2006.
Vibrationally Excited Molecules: the nonlinear mechanical approach
by **S. C. Farantos**$^*$.

[54] International Conference of Computational Methods in Sciences
and Engineering 2006 (ICCMSE 2006)
HOTEL PANORAMA, Chania-Crete, Greece, 27 October - 1 November, 2006.
Periodic Orbits in Biological Molecules: Phase Space Structures and Selectivity
by **S. C. Farantos**$^*$.

[55] Nonlinear Dynamics of Acoustic Modes in Finite Lattices
International workshop on Localization, Equipartition, Transport
MPI PKS Dresden, Germany, December 6 - 8, 2006
Searching for localized motions in biological molecules: Phase space structures and selectivity
by **S. C. Farantos**$^*$.

[56] 20th International Conference and Summer School
NONLINEAR SCIENCE AND COMPLEXITY
Patra, July 19-31, 2007.
Non-Linear Vibrational Normal Modes of Biomolecules
by **S. C. Farantos**$^*$.

[57] International Conference of Computational Science and
its Applications (ICCSA 2007)
26-29 August 2007, Sunway Hotels and Resorts,
Kuala Lumpur, Malaysia.
Non-Linear Vibrational Normal Modes of Biomolecules
by **S. C. Farantos**$^*$.

[58] International Conference of Computational Methods in Sciences
and Engineering 2007 (ICCMSE 2007)

HOTEL MARBELLA, Corfu, Greece, 25-30 September 2007.
Protein dynamics and spectroscopy for ferryl intermediate of Cytochrome c Oxidase:
A molecular dynamics approach
by Vangelis Daskalakis, Stavros C. Farantos, and Constantinos Varotsis.

[59] 21th International Conference and Summer School
NONLINEAR SCIENCE AND COMPLEXITY
Athens, July 21- August 2, 2008.
Energy Localization in Large Molecules and Large Scale Computations on Grid Infrastructures
by **S. C. Farantos**$^*$.

[60] COST (GRIDCHEM) Training School on Molecular and
Material Science GRID Applications:
An EU-IndiaGrid/CompChem hands-on tutorial
Trieste, ICTP Adriano Guesthouse, 15-18 September 2008.
GRID Molecular Dynamics: A multiple shooting algorithm
for an extended phase space sampling and long time dynamics
by **S. C. Farantos**$^*$.

[61] The International Conference on The Theory and
Applications of Computational Chemistry in 2008 (TACC2008),
23-27 September 2008, Shanghai, China.
Interpreting Molecular Vibrational Spectra by Periodic Orbits
by **S. C. Farantos**.

[62] International Conference of Computational Methods in Sciences
and Engineering 2008 (ICCMSE 2008),
Hotel Belveder Imperial, Hersonissos, Crete, Greece, 25-30 September 2008.
A parallel code for solving the molecular Time Dependent Schrödinger
Equation in Cartesian coordinates
by **J. Suarez**, S. Stamatiadis, S. C. Farantos, L. Lathouwers.

[63] Conference on Bifurcations (BIFR08):
Mathematical and Quantum Aspects and Applications,
Madrid, 9-12 December, 2008.
Bifurcations of Molecular Vibrations:
Discovery of New Types of Motion, Localized states and Reaction Paths
by **S. C. Farantos**$^*$.

[64] XVI Symposium on High Resolution Molecular Spectroscopy (HighRus2009),
Lake Baikal, Irkutsk, Russia, July 5-10, 2009.
Energy localization and bifurcation phenomena in vibrationally excited molecules
by **S. C. Farantos**$^*$.

[65] Quantum Systems in Chemistry and Physics XIV (QSCP XIV),
San Lorenzo del Escorial, Madrid, Spain, September 13-19, 2009.

Bifurcation phenomena in vibrationally excited small and
large molecules and their spectrocopic signatures
by **S. C. Farantos**[*].

[66] EGEE'09,
Barcelona, Spain, September 13-19, 2009.
Quantum Grid Dynamics (QGD): a method for solving the molecular
Schroedinger Equation in Cartesian coordinates via
angular momentum projection operators
by **S. C. Farantos**[*].

[67] Ultrafast dynamics and structure: towards biological and
biomedical applications
Marie Curie chair and ESF summer school 2009,
Rhodes, Greece, September 29th - October 3rd, 2009.
Energy Localisation in Molecules, Bifurcation Phenomena,
and their Spectroscopic Signatures
by **S. C. Farantos**[*].

[68] 5th EGEE User Forum, Uppsala, April 12-15, 2010.
Protein Molecular Dynamics and Free Energy Calculations
on the EGEE Production Grid
by **Stavros C. Farantos**[*], Daskalakis Vangelis, Giatromanolakis Manos,
Porrini Massimiliano and Gervasi Osvaldo.

[69] SDMC 2011: Spectroscopy and Dynamics of Molecules and Clusters,
Cobertt, India, February 18-20, 2011.
Non-linear molecular dynamics for understanding spectroscopy and chemical reactivity
by **Stavros C. Farantos**[*].

[*] *Invited talk.*

**SEMINARS**

[1] International Seminar on Molecular Physics and
Biophysics of Water Systems 1993 - 1994.
The Mendeleev Chemical Society and Institute of
Physics, St. Petersburg State University.
St. Petersburg, Russia, April 27, 1994.
*The Cubic Structures of Water Clusters,*
by **S. C. Farantos.**

[2] Seminar at :
Democritos:

Athens, June 15th, 1994.
*Small Clusters of Water Molecules,*
by **S. C. Farantos.**

[3] Seminar at :
Laboratoire de Photophysique Moleculaire du CNRS:
Orsay, Paris, France, June 23rd, 1995.
*Potential Functions and Dynamics of* $Mg^{m+}Ar_n$ *Clusters.*
by **S. C. Farantos.**

[4] Seminar at :
University of Heildeberg, Department of Chemistry
Heildeberg, Germany, December 18th, 1995.
*The Method of Periodic Orbits for Extracting the Dynamics from Vibrational Spectra*
by **S. C. Farantos.**

[5] Seminar at :
Pacific Northwest National Laboratory-EMSL:
Theory, Modeling and Simulation
Richland, July, 1996.
*Structure and Dynamics of Molecules and Clusters.*
by **S. C. Farantos.**

[6] Seminar at :
Democritos: Institute of Physical Chemistry
Athens, November 8th, 1996.
*Structure and Dynamics of Molecules and Clusters:*
An approximation through the geometry of phase space.
by **S. C. Farantos.**

[7] Seminar at :
Max-Planck-Institute: Institute für Strömungsforschung,
Göttingen, Germany, October 1st, 1997
$Mg^+(Sr^+)$ *Clusters: Structures, Spectroscopy, Isomerizations.*
by **S. C. Farantos.**

[8] Seminar at :
University College London (UCL):
Department of Physics and Astronomy,
London, UK, February 3, 1999
*Periodic Orbits Continuation/Bifurcation Diagrams*
*for Exploring Molecular Dynamics and Spectroscopy.*
by **S. C. Farantos.**

[9] Seminar at :
Massachusetts Institute of Technology (MIT):

Department of Chemistry,
Boston, USA, March 18, 1999
*Periodic Orbits Continuation/Bifurcation Diagrams*
*for Exploring Molecular Dynamics and Spectroscopy.*
by **S. C. Farantos.**

[10] Seminar at :
Pacific Northwest National Laboratory:
Environmental Molecular Science Laboratory (EMSL-PNNL),
Richland, Washington State, USA, March 30, 1999
*Periodic Orbits Continuation/Bifurcation Diagrams*
*for Exploring Molecular Dynamics and Spectroscopy.*
by **S. C. Farantos.**

[11] Seminar at :
Dept. of Chemistry, University of Bonn:
Bonn, Germany, November 2nd, 2000
*Variable Finite Difference Methods for solving*
*the Schrödinger Equations in Molecular Dynamics.*
by **S. C. Farantos.**

[12] Seminar at :
Max-Planck-Institute:
Institute für Strömungsforschung,
Göttingen, Germany, November 8th, 2000
*Variable Finite Difference Methods for solving*
*the Schrödinger Equations in Molecular Dynamics.*
by **S. C. Farantos.**

[13] Seminar at :
ETH Zurich, Department of Physical Chemistry,
Zurich, Swiss, September 7th, 2001
*Saddle Node States in Chemistry, Biology and Physics.*
by **S. C. Farantos.**

[14] Seminar at :
Dept. of Chemistry, University of Bonn:
Bonn, Germany, December 3d, 2001
*Saddle Node States in Chemistry, Biology and Physics.*
by **S. C. Farantos.**

[15] Seminar at :
Dept. of Chemistry, University of Illinois at Urbana:
Champagn-Urbana, Illinois USA, October 2nd, 2002
*Exploring Elementary Chemical Processes by Bifurcation Diagrams of Periodic Orbits.*
by **S. C. Farantos.**

[16] Seminar at :
Dept. of Chemistry, University of Western Ontarion Canada:
London-Ontario, Canada, October 9th, 2002
*Exploring Elementary Chemical Processes by Bifurcation Diagrams of Periodic Orbits.*
by **S. C. Farantos.**

[17] Seminar at :
Dept. of Chemistry, University of Toronto:
Toronto, Canada, October 11th, 2002
*Exploring Elementary Chemical Processes by Bifurcation Diagrams of Periodic Orbits.*
by **S. C. Farantos.**

[18] Seminar at :
Max Planck Istitut für Physik Complexer Systeme-Dresden, Germany, January 21st, 2003
*Exploring Elementary Chemical Processes by Bifurcation Diagrams of Periodic Orbits.*
by **S. C. Farantos.**

[19] Seminar at :
National Research Foundation, Athens, Greece, March 30th, 2004
*Order and Chaos in forming and breaking Chemical Bonds.*
by **S. C. Farantos.**

[20] Seminar at :
University of Reims, GSMA, Reims, France, June 15, 2007
*Bifurcations and Localization in Highly Vibrationally Excited Molecules.*
by **S. C. Farantos.**

[21] Seminar at :
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH (IISER) MOHALl,
February 22, 2011
*How does a chemical bond break? Non-linear molecular dynamics*
*for understanding chemical reactivity.*
by **S. C. Farantos.**

[22] Seminar at :
Department of Chemistry, University of Crete, Heraklion, Crete,
March 11, 2011
*How does a chemical bond break? New theories for studying chemical reactivity*
by **S. C. Farantos.**

[23] Seminar at :
Department of Chemistry, University of Crete, Heraklion, Crete,
December 09, 2011
*New Computational Technologies for Molecular Dynamics:*
*GRID - how to use planet Earths computers*

by **S. C. Farantos.**

[24] Seminar at :
Department of Chemistry, Technical University of Munich, MUnich, December 05, 2012
*Nonlinear Mechanics applied to Molecular Dynamics: for understanding chemical reactions*
by **S. C. Farantos.**

## GRANTS

[1] *Chemical Dynamics of Small Molecules: Intramolecular Dynamics and Chemical Reactions*, with Jonathan Tennyson (University College).
Stimulation, Contract No: ST2J-0143-1-GR(TT), 47276 ECU, 1986-1988.

[2] *Theoretical Investigations in Two-dimensional Nonlinear Lattice Systems. Dynamical Studies of Small Clusters*,
with S. Pnevmatikos (Research Center of Crete), N. Flytzanis (University of Crete), M. Remoissenet (University of Dijon), and H. Büttner and F.G. Martens (Univerisity of Bayreuth).
Stimulation, Contract No: GR06PUJU1, 94980 ECU, 1985-1988.

[3] J.S.P. and ERASMUS (Educational Program),
with C. Fotakis, approx. 5000 ECU per annum, 1985-1987.

[4] NATO Travel Grant,
with D. R. Crosley (SRI), and R.J. Donovan (University of Endiburg), 1987-1989.

[5] *Understanding Solvation Effects in Chemistry Through the Study of Microsolvent Clusters,*
with P. Brechignac (University of Paris-Sud), A. J. Stace (University of Sussex).
Science Contract No: SC1*0331-C(EDB), 202 500 ECU, 1991-1993.

[6] *Vibrational Spectra and Dynamics of Molecules with Chaotic Classical Behaviour,*
with Howard S. Taylor (University of Southern California), 1991-1992.
NATO Travel Grant SA. 9-15-02(CRG.901052), 150000 Belgian Francs.

[7] *Classical and Quantum Studies of Dynamical Systems with 3 Degrees of Freedom,*
with George Contopoulos, University of Athens, 1991-1993.
2382 ()68, 6.796.000 Dr.

[8] *New States of Highly Excited Molecules for Promoting Chemical Reactions,*
with Tino Borondo,Universidad Autonoma de Madrid, 1994-1995.
Bilateral Cooperation with Spain, 1.300.000 Dr.

[9] *A Study of Solvation Effects: Clusters of Magnesium - Argon and Aniline - Argon,*
with M. Velegrakis and Ph. Brechignac (Orsay), 1995.
Bilateral Cooperation with France, 560.000 Dr.

[10]*A Study of Solvation Effects: Clusters of Magnesium - Argon and Aniline - Argon,*

with M. Velegrakis and Ph. Brechignac (Orsay), 1996.
Bilateral Cooperation with France, 700.000 Dr.

[11]*Chemical Dynamics: Theoretical and Experimental Study of Atomic and Molecular Clusters,*
with M. Velegrakis, S. Xantheas (PNL-USA), and I. Samios (Univ. of Athens), 1996-98.
PENED 8.000.000 Dr.

[12]*Unimolecular decay of van der Waals clusters: the role of dynamical correlations and chaos,*
with A. J. Stace (Univ. of Sussex) and D. Trubnikov (Moscow State Univ.), 1997-99.
INTAS 4800 ECU.

[13]*Applied Molecular Spectroscopy: a postgraduate program,*
with the Department of Chemistry of Univ. of Athens and the
the Department of Chemical Engineering of Univ. of Patras, 1998-2000.
EPEAEK 291,353,000 Drachmas.

[14]*Spectroscopy and Dynamics of Vibrationally Highly Excited Molecules*
with Dr. Reinhard Schinke, MPI für Strömungsforschung, 1998-2000.
Alexander von Humboldt Foundation, 30000 DM.

[15]*Investigation of Water Nucleation under*
*Conditions of Radioactive Contamination of the Atmosphere*
with Dr. Alice Vegiri (NHRF) and
Prof. Sergey Chevkounov, St. Petersburg State Technical University, 1999-2000.
NATO Linkage Grant SST.CLG 974515. 12500 $ US.

[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 clustres*
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]*Hrakleitos*: PhD scholarship, Ministry of Education,
*Study of elementary chemical reactions of biological molecules with non-linear 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-COMPCHEM),
2006-2010, 720842 Euros.

[23]*FP7-PEOPLE-2007-4-3-IRG*: Development of ab initio based classical interaction potentials for the study of the structure and dynamics of aqueous solutions and interfaces (SIMULAQI),
2007-2010, 75000 Euro.

**PhD Thesis Supervision**

[1] Manolis Founargiotakis.
*Study of Chemical Dynamics with Periodic Orbits*,
July 1989.

[2] Alice Vegiri.
*Potential Energy Surfaces and Dynamics of the Excited* $OH(A^2\Sigma^+)$ *in Collisions with He and* $CO(X^1\Sigma^+)$,
March 1989.

[3] Aristea Prosmiti.
*Study of the Spectroscopy and Dynamics of Triatomic and Tetratomic Molecules with the Periodic Orbit Method (POM).*
February 1996.

[4] George Fanourgakis.
*Study of Metal Ion - Inert Gas Clusters:* $Mg^+Ar_n$, $Sr^+Ar_n$.
November 1999.

[5] Stamatis Stamatiadis.
*Saddle-Node Bifurcations in the Vibrational Spectra of Small Polyatomic Molecules.*
May 2003.

[6] Andreas Mavrantonakis
*Studies of Elementary Chemical Processes by Quantum and Classical Mechanical Techniques*

November 2006.

### MS Thesis

[1] Stavros Kapetanakis.
*Water Clusters.*
August 1997.

[2] Apostolos Hatzopoulos.
*Studies of Time Dependent Models with the Finite Difference Method.*
September 2002.

[3] Erofili Filippou.
*An Ab Initio Quantum Mechanical Study of the Photofragmentation Spectra of $Sr^+CO$ complex.*
September 2002.

[4] Alexandros Kampanarakis.
*Temperature Dependence of Vibrational Spectra of Cytochrome c Oxidase*
September 30, 2008.

### Diplomas

[1] Anastasios I. Nezis.
*Exploring Molecular Phase Space.*
January 1994.

[2] Iwannis R. Papadakis.
*Methods for Locating Minima in Atomic and Molecular Clusters.*
February 1995.

### Postdoctoral Fellows

[1] Vangelis Daskalakis
September 2006 - May 2010

[2] Jaime Suarez
November 2006 - October 2009

[3] Massimiliano Porrini

February 2007 - January 2010

[4] Frederic Mauguiere
December 2009 - November 2010