

# 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*

## 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 up to 2004

[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]

### Articles in Books after invitation up to 2004

[96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107]

### Articles in International Journals 2005 - 2012

[108, 109, 110, 111, 112, 113, 114, 115, 116]

[117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129]

### Articles in Books after invitation up to 2005 - 2012

[130, 131, 132, 133, 134, 135, 136, 137]

**Books in English**

[138]

**Books Translated in Greek**

[139, 140]

**ADDRESS**

**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

- [1] **S. Farantos**, E.C. Leisegang, J. N. Murrell, K. Sorbie, J.J.C. Teixeira-Dias, and A.J.C. Varandas.  
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. [1](#)
- [2] J. N. Murrell, and **S. Farantos**.  
An Analytical Function for the Potential Energy Surface of Ozone.  
*Mol. Phys.*, 34(4):1185–1188, 1977. [1](#)
- [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. [1](#)
- [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. [1](#)
- [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. [1](#)
- [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. [1](#)
- [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. [1](#)
- [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. [1](#)
- [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. [1](#)

- [10] **S. C. Farantos**.  
Exponentially Divergent Trajectories and RRKM Behaviour of  $Ar_3$  Clusters.  
*Chem. Phys. Letters*, 92:379–382, 1982. [1](#)
- [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. [1](#)
- [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. [1](#)
- [13] **S. C. Farantos**.  
Studies on the Statistical Behaviour of  $Ar$  Clusters: The  $Ar_4$  Case.  
*J. Phys. Chem.*, 87:5061–5064, 1983. [1](#)
- [14] G. Theodorakopoulos, **S. C. Farantos**, R. J. Buenker, and S. D. Peyerimhoff.  
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. [1](#)
- [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. [1](#)
- [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. [1](#)
- [17] **S. C. Farantos**.  
A Quasiclassical Study of Collisions of  $He$  with  $HD(B^1\Sigma_u^+)$ .  
*Mol. Phys.*, 54(4):835–845, 1985. [1](#)
- [18] **S. C. Farantos**, and J. Tennyson.  
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. [1](#)
- [19] **S. C. Farantos**, and J. Tennyson.  
Quantum and Classical Vibrational Chaos in Floppy Molecules.  
*J. Chem. Phys.*, 82(2):800–809, 1985. [1](#)

- [20] J. Tennyson, and **S. C. Farantos**.  
Routes to Vibrational Chaos in Triatomic Molecules.  
*Chem. Phys.*, 93(2):237–244, 1985. [1](#)
- [21] J. Tennyson, G. Brocks, and **S. C. Farantos**.  
Transition Intensities and Fluorescence Lifetimes for Regular and Chaotic States of *LiCN*.  
*Chem. Phys.*, 104:399–407, 1986. [1](#)
- [22] **S. C. Farantos**.  
Chaotic Structure in the Phase Space of Acetylene.  
*J. Chem. Phys.*, 85(1):641–642, 1986. [1](#)
- [23] **S. C. Farantos**, and J. Tennyson.  
On the Vibrational Born–Oppenheimer Separation Scheme for Molecules with Regular and Chaotic States.  
*J. Chem. Phys.*, 84(11):6210–6217, 1986. [1](#)
- [24] **S. C. Farantos**.  
A Classical Trajectory Study of the Reaction  $He(^1S) + H_2(B^1\Sigma_u^+) \rightarrow HeH(A^2\Sigma^+) + H(^2S)$ .  
*Mol. Phys.*, 59(6):1273–1275, 1986. [1](#)
- [25] **S. C. Farantos**.  
Potential Energy Surface; A Fundamental Concept for Studying Chemical Dynamics (in Greek).  
*Chimica Chronica, New Series*, 16:107–122, 1987. [1](#)
- [26] **S. C. Farantos**, and N. Flytzanis.  
Classical Mechanical Analysis of Vibrational Dephasing and Rotational Energy Redistribution in *CO – Ar*.  
*J. Chem. Phys.*, 87(11):6449–6456, 1987. [1](#)
- [27] M. Founargiotakis, **S. C. Farantos**, and J. Tennyson.  
Regular/Irregular Phase Space Structure of *HCN/HNC*.  
*J. Chem. Phys.*, 88(3):1598–1607, 1988. [1](#)
- [28] A. Vegiri, and **S. C. Farantos**.  
Ab Initio Potential Energy Surfaces of  $He(^1S) + OH(X^2\Pi)$  and  $He(^1S) + OH(A^2\Sigma^+)$ .  
*J. Phys. Chem.*, 92:2723–2728, 1988. [1](#)
- [29] **S. C. Farantos**, and A. Vegiri.  
Quantum Mechanical Study of Rotational Inelastic Collisions of  $He + OH(A^2\Sigma^+)$  Excited Potential Energy Surface.  
*J. Phys. Chem.*, 92:2719–2723, 1988. [1](#)
- [30] A. D. Mistriotis, N. Flytzanis, and **S. C. Farantos**.  
Potential Model for Silicon Clusters.  
*Phys. Rev. B*, 39(2):1212–, 1989. [1](#)

- [31] M. Founargiotakis, **S. C. Farantos**, G. Contopoulos, and C. Polymilis. Periodic Orbits, Bifurcations and Quantum Mechanical Eigenfunctions and Spectra. *J. Chem. Phys.*, 91(1):1389–1402, 1989. 1
- [32] **S. C. Farantos**, M. Founargiotakis, and C. Polymilis. Study of Molecular Phase Space Structure Through Families of Periodic Orbits. *Chem. Phys.*, 135:347–356, 1989. 1
- [33] A. Vegiri, and **S. C. Farantos**. A Classical Dynamical Investigation of the Mechanism of Electronic Quenching of  $OH(A^2\Sigma^+)$  in Collisions with  $CO(X^1\Sigma^+)$ . *Mol. Phys.*, 69(1):129–146, 1990. 1
- [34] **S. C. Farantos**, and M. Founargiotakis. Wave Packet Dynamics and Phase Space Structure of  $HCN$  Molecule. *Chem. Phys.*, 142:345–359, 1990. 1
- [35] **S. C. Farantos**, J. M. Gomez Llorente, O. Hahn, and H. S. Taylor. The Extraction of Dynamics from Spectra in Regions of Mixed Chaotic and Regular Motion: The  $HCN$  Case. *Chem. Phys. Letters*, 166(1):71–76, 1990. 1
- [36] A. Vegiri, and **S. C. Farantos**. 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. 1
- [37] J. M. Gomez Llorente, **S. C. Farantos**, O. Hahn, and H. S Taylor. Classical Mechanical Methods for Extracting the Dynamics from Stimulated-Emission Pumping Spectra. *J. Opt. Soc. Am. B*, 7(9):1851–1858, 1990. 1
- [38] **S. C. Farantos**, J. M. Gomez Llorente, O. Hahn, and H. S. Taylor. 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. 1
- [39] **S. C. Farantos**, J. M. Gomez Llorente, O. Hahn, and H. S. Taylor. Classical Dynamical Analysis of the Vibrational Spectra for Small Polyatomic Molecules. *Int. J. Quantum Chem.*, 24:429–446, 1990. 1
- [40] **S. C. Farantos**, and H. S Taylor. The Photodissociation of  $O_3$ : A Classical Dynamical Approach for the Interpretation of the Recurrences in the Autocorrelation Function. *J. Chem. Phys.*, 94(7):4887–4895, 1991. 1

- [41] **S. C. Farantos**, J. M. Gomez Llorente, O. Hahn, and H. S. Taylor.  
On the Consistency Between Recent Experimental Results and a Previous  
Theoretical Analysis of *HCN/HNC*.  
*J. Chem. Phys.*, 94(1):2376, 1991. 1
- [42] L. Zachilas, and **S. C. Farantos**.  
Periodic Orbits and Quantum Localization in the van der Waals System  
*CO – Ar*.  
*Chem. Phys.*, 154:55–62, 1991. 1
- [43] **S. C. Farantos**.  
The Importance of Periodic Orbits in Analysing Photodissociation Reso-  
nances: the  $O_3$  Case.  
*Chem. Phys.*, 159:329–338, 1992. 1
- [44] A. Vegiri, and **S. C. Farantos**.  
Classical Dynamics of Hydrogen Bonded Systems: Water Clusters.  
*J. Chem. Phys.*, 98(5):4059–4075, 1993. 1
- [45] **S. C. Farantos**.  
Periodic Orbits as a Probe to Reveal Exotic States: The Saddle-Node  
States.  
*Laser Chemistry*, 13:87–99, 1993. 1
- [46] **S. C. Farantos**, and L. Zachilas.  
Testing Molecular Potential Functions with Bifurcation Diagrams of Pe-  
riodic Orbits .  
*Mol. Phys.*, 80(6):1499–1505, 1993. 1
- [47] **S. C. Farantos**, S. Kapetanakis, and A. Vegiri.  
Minimum Structures and Dynamics of Small Water Clusters.  
*J. Phys. Chem.*, 97:12158–12166, 1993. 1
- [48] B. R. Eggen, A. J. Marks, J. N. Murrell, and **S. C. Farantos**.  
Water Clusters - a speculation.  
*Chem. Phys. Letters*, 219:247–251, 1994. 1
- [49] **S. C. Farantos**.  
Water Clusters: The  $(H_2O)_{64}$  case.  
*Z. Phys. D*, 31:213–217, 1994. 1
- [50] R. Prosmi, **S. C. Farantos**, and H. S. Taylor.  
A Periodic Orbit Approach to Spectroscopy and Dynamics of  $SO_2$  :  
 $\tilde{C}^1B_2 \rightarrow \tilde{X}^1A_1$ .  
*Mol. Phys.*, 82(6):1213–1232, 1994. 1
- [51] G. Contopoulos, **S. C. Farantos**, H. Papadaki, and C. Polymilis.  
Complex Unstable Periodic Orbits and their Manifestation in Classical  
and Quantum Dynamics.  
*Phys. Rev. E*, 50(5):4399–4403, 1994. 1

- [52] **S. C. Farantos.**  
Methods for Locating Periodic Orbits in Highly Unstable Systems.  
*THEOCHEM J. Mol. Struct.*, 341:91–100, 1995. [1](#)
- [53] R. Prosmi, and **S. C. Farantos.**  
Periodic Orbits, Bifurcation Diagrams and the Spectroscopy of C<sub>2</sub>H<sub>2</sub> System.  
*J. Chem. Phys.*, 103(9):3299–3314, 1995. [1](#)
- [54] R. Prosmi, **S. C. Farantos**, R. Guantes, F. Borondo, and R. M. Benito.  
A Periodic Orbit Analysis of the Vibrationally Highly Excited LiNC/LiCN:  
a comparison with quantum mechanics.  
*J. Chem. Phys.*, 104(8):2921–2931, 1996. [1](#)
- [55] G. S. Fanourgakis, and **S. C. Farantos.**  
Potential Functions and Static and Dynamic Properties of Mg<sup>m+</sup>Ar<sub>n</sub>, m = 1, 2; n = 1 – 18 clusters.  
*J. Phys. Chem.*, 100:3900–3909, 1996. [1](#)
- [56] **S. C. Farantos.**  
Exploring Molecular Vibrations with Periodic Orbits.  
*Int. Rev. Phys. Chem.*, 15(2):345–374, 1996. [1](#)
- [57] **S. C. Farantos**, Hans-Martin Keller, R. Schinke, K. Yamashita, and K. Morokuma.  
Normal Mode and Isomerization Bending States in HCP:  
Periodic Orbit Assignment and Spectroscopic Signature.  
*J. Chem. Phys. (Communication)*, 104(24):10055–10058, 1996. [1](#)
- [58] J. Papadakis, G. S. Fanourgakis, M. Founargiotakis, and **S. C. Farantos.**  
Comparison of Line Search Minimization Algorithms for Exploring Topography of Multidimensional Potential Energy Surfaces: Mg<sup>+</sup>Ar<sub>n</sub> case.  
*J. Comput. Chem.*, 18:1011–1022, 1997. [1](#)
- [59] G. S. Fanourgakis, **S. C. Farantos**, P. Parneix, and Ph. Bréchnignac.  
An Effective Transition State for a Complex Cluster Isomerization Process: comparison between anharmonic and harmonic models for Mg<sup>+</sup>Ar<sub>12</sub>.  
*J. Chem. Phys.*, 106(12):4954–4962, 1997. [1](#)
- [60] M. Founargiotakis, **S. C. Farantos**, H. Skokos, and G. Contopoulos.  
Bifurcation Diagrams of Periodic Orbits for Unbound Molecular Systems: FH<sub>2</sub> .  
*Chem. Phys. Letters*, 277:456–464, 1997. [1](#)
- [61] Ch. Beck, Hans-Martin Keller, S. Yu. Grebenshchikov, R. Schinke, **S. C. Farantos**, K. Yamashita, and K. Morokuma.



- Highly Excited Vibrational States of HCP and their Analysis in Terms of Periodic Orbits: The genesis of saddle-node states and their spectroscopic signature.  
*J. Chem. Phys.*, 107(23):9818–9834, 1997. [1](#)
- [62] S. S. Xantheas, G. S. Fanourgakis, **S. C. Farantos**, and M. Velegarakis. Spectroscopic Constants of the  $X^2\Sigma^+$  and  $A^2\Pi$  States of  $\text{Sr}^+\text{Ar}$  from First Principles: Comparison with experiment.  
*J. Chem. Phys.*, 108(1):46–49, 1998. [1](#)
- [63] **S. C. Farantos**. POMULT: A Program for Computing Periodic Orbits in Hamiltonian Systems Based on Multiple Shooting Algorithms.  
*Comp. Phys. Comm.*, 108:240–258, 1998. [1](#)
- [64] S. Yu. Grebenshchikov, C. Beck, R. Schinke, and **S. C. Farantos**. Three-Dimensional Molecular Wave Packets: Calculation of Revival Times from Periodic Orbits.  
*Phys. Letters A*, 243:208–214, 1998. [1](#)
- [65] G. S. Fanourgakis, **S. C. Farantos**, M. Velegarakis, and S. S. Xantheas. Photofragmentation Spectra and Structures of  $\text{Sr}^+\text{Ar}_n$ ,  $n = 2–8$  Clusters: Experiment and Theory.  
*J. Chem. Phys.*, 109(1):108–120, 1998. [1](#)
- [66] M. Velegarakis, G. E. Froudakis, and **S. C. Farantos**. Stability and Structure of  $\text{Ni}^+\text{Ar}_n$  and  $\text{Pt}^+\text{Ar}_n$  Clusters.  
*J. Chem. Phys.*, 109(11):4687–4688, 1998. [1](#)
- [67] G. E. Froudakis, G. S. Fanourgakis, **S. C. Farantos**, and S. S. Xantheas. Binding Energies and Structures of  $\text{C}^+\text{Ar}_n$ , ( $n=1-5$ ), Clusters from First Principles.  
*Chem. Phys. Letters*, 294:109–116, 1998. [1](#)
- [68] **S. C. Farantos**, C. Beck, and R. Schinke. Periodic Orbits and Vibrational Wave Functions for DCP: nonlinear resonances in isotopically substituted molecules.  
*Theor. Chem. Acc.*, 100:147–153, 1998. [1](#)
- [69] Pankaj Bhatia, Biswajit Maiti, N. Sathyamurthy, S. Stamatiadis, and **S. C. Farantos**. Exploring Molecular Motions in Collinear  $\text{HeH}_2^+$  and its isotopic Variants Using Periodic Orbits.  
*PCCP*, 1:1105–1113, 1999. [1](#)
- [70] G. S. Fanourgakis, **S. C. Farantos**, Ch. Lüder, M. Velegarakis, and S. S. Xantheas. Photofragmentation Spectra and Potential Energy Surfaces of  $\text{Sr}^+\text{Ar}_2$ .  
*PCCP*, 1:977–981, 1999. [1](#)

- [71] M. Velegrakis, G. E. Froudakis, and **S. C. Farantos**,  
Coordination of Ti Cation Embedded in Argon Clusters.  
*Chem. Phys. Letters*, 302:595–601, 1999. [1](#)
- [72] R. Prosimiti, **S. C. Farantos**, and H. Guo.  
Assigning the Transition from Normal to Local Vibrational Mode in SO<sub>2</sub>  
by Periodic Orbits.  
*Chem. Phys. Letters*, 311:241–247, 1999. [1](#)
- [73] H. Ishikawa, R. W. Field, **S. C. Farantos**, M. Joyeux, J. Koput, C. Beck,  
and R. Schinke.  
HCP - CPH Isomerization: Caught in the Act. *Ann. Rev. Phys. Chem.*,  
50:443–484, 1999. [1](#)
- [74] R. Guantes, and **S. C. Farantos**.  
High Order Finite Difference Algorithms for Solving the Schrödinger  
Equation in Molecular Dynamics.  
*J. Chem. Phys.*, 111(24):10827–10835, 1999. [1](#)
- [75] R. Guantes, A. Nezis, and **S. C. Farantos**.  
Periodic Orbit - Quantum Mechanical Investigation of the Inversion Mech-  
anism of Ar<sub>3</sub>.  
*J. Chem. Phys.*, 111(24):10836–10842, 1999. [1](#)
- [76] J. Weish, J. Hauschildt, R. Düren, R. Schinke, J. Koput, S. Stamatiadis,  
and **S. C. Farantos**.  
Saddle-node Bifurcations in the Spectrum of HOCl.  
*J. Chem. Phys.*, 112(1):77–93, 2000. [1](#)
- [77] S. Stamatiadis, R. Prosimiti, and **S. C. Farantos**.  
AUTO\_DERIV: Tool for automatic differentiation of a FORTRAN code.  
*Comp. Phys. Comm.*, 127:343–355, 2000. [1](#)
- [78] Biswajit Maiti, N. Sathyamurthy, S. Stamatiadis, and **S. C. Farantos**,  
Periodic Orbit Analysis for HeH<sub>2</sub><sup>+</sup> in Three Dimensions.  
*Indian Journal of Chemistry A*, 39A:338–344, 2000. [1](#)
- [79] G. E. Froudakis, **S. C. Farantos**, and M. Velegrakis, .  
Mass Spectra and Theoretical Modeling of Li<sup>+</sup>Ne<sub>n</sub>, Li<sup>+</sup>Ar<sub>n</sub> and Li<sup>+</sup>Kr<sub>n</sub>  
Clusters.  
*Chem. Phys.*, 258:13–20, 2000. [1](#)
- [80] J. Bredenbeck, C. Beck, R. Schinke, J. Koput, S. Stamatiadis, **S. C.**  
**Farantos**, and M. Joyeux.  
The Vibrational Spectrum of Deuterated Phosphaethyn: A quantum me-  
chanical, classical and semiclassical analysis.  
*J. Chem. Phys.*, 112(20):8855–8865, 2000. [1](#)

- [81] A. Vegiri, and **S. C. Farantos**.  
Cluster Collisions of Water Tetramers: A classical dynamical study.  
*Chem. Phys.*, 262:337–347, 2000. [1](#)
- [82] R. Guantes, and **S. C. Farantos**.  
High Order Finite Difference Algorithms for Solving the Schrödinger Equation in Molecular Dynamics. II. Periodic variables.  
*J. Chem. Phys.*, 113(23):10429–10437, 2000. [1](#)
- [83] M.N. Vrahatis, A.E. Perdiou, V.S. Kalantonis, E.A. Perdios, K. Papadakis, R. Prosmiiti, and **S. C. Farantos**.  
Application of the Characteristic Bisection Method for Locating and Computing Periodic Orbits in Molecular Systems.  
*Comp. Phys. Comm.*, 138:53–68, 2001. [1](#)
- [84] S. Stamatiadis, **S. C. Farantos**, H.-M. Keller, and R. Schinke.  
Saddle node states in the spectra of HCO and DCO: a periodic orbit classification of vibrational levels.  
*Chem. Phys. Letters*, 344:565–572, 2001. [1](#)
- [85] R. Guantes, and **S. C. Farantos**.  
Reply to the comment “High Order Finite Difference Algorithms for Solving the Schrödinger Equation in Molecular Dynamics”.  
*J. Chem. Phys.*, 115(14):6796–6797, 2001. [1](#)
- [86] G. E. Froudakis, M. Mühlhäuser, **S. C. Farantos**, A. Sfounis, and M. Velegarakis.  
Mass Spectra and Structures of  $\text{Cu}^+\text{Rg}_n$  Clusters ( $\text{Rg} = \text{Ne}, \text{Ar}$ ).  
*Chem. Phys.*, 280:43–51, 2002. [1](#)
- [87] 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.*, 106 (feature article):5407–5421, 2002. [1](#)
- [88] Rüdiger Siebert, Paul Fleurat-Lessard, R. Schinke, Martina Bittererová, 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. [1](#)
- [89] **S. C. Farantos**, E. Filippou, S. Stamatiadis, G. E. Froudakis, M. Mühlhäuser, M. Massauti, A. Sfounis, and M. Velegarakis.  
Photofragmentation Spectra of  $\text{Sr}^+\text{CO}$  Complex: experiment and ab initio calculations.  
*Chem. Phys. Letters*, 366:231–237, 2002. [1](#)

- [90] R. Prosimiti, and **S. C. Farantos**.  
 Periodic Orbits and Bifurcation Diagrams of Acetylene/Vinylidene Revisited.  
*J. Chem. Phys.*, 118(18):8275–8280, 2003. [1](#)
- [91] T. Azzam, R. Schinke, **S. C. Farantos**, M. Joyeux, and K. A. Peterson.  
 The Bound State Spectrum of HOBr up to Dissociation Limit: Evolution of saddle-node bifurcations.  
*J. Chem. Phys.*, 118(21):9643–9652, 2003. [1](#)
- [92] **S. C. Farantos**, E. Filippou, S. Stamatiadis, G. E. Froudakis, M. Mühlhäuser, M. Peric, M. Massaouti, A. Sfounis, and M. Velegarakis.  
 The Excited States of  $\text{Sr}^+\text{CO}$ : photofragmentation spectra and *ab initio* calculations.  
*Chem. Phys. Letters*, 379:242–247, 2003. [1](#)
- [93] Z.W. Qu, H. Zhu, M. Tashiro, R. Schinke, and **S. C. Farantos**.  
 The Huggins band of ozone: Unambiguous electronic and vibrational assignment.  
*J. Chem. Phys. (Communication)*, 120(15):6811–6814, 2004. [1](#)
- [94] **S. C. Farantos**, Shi Ying Lin, and Hua Guo.  
 A regular isomerization path among chaotic vibrational states of  $\text{CH}_2(\tilde{a}^1A_1)$ .  
*Chem. Phys. Letters*, 399:260–265, 2004. [1](#)
- [95] Z.W. Qu, H. Zhu, R. Schinke, and **S. C. Farantos**.  
 The Huggins band of ozone: A theoretical analysis.  
*J. Chem. Phys.*, 121(23):11731–11745, 2004. [1](#)
- [96] J. Tennyson, and **S. C. Farantos**.  
 Quantum and Classical Vibrational Chaos in Small Molecules.  
*NewsLetters in Heavy Particle Dynamics - CCP6*, 9:39–41, 1986. [1](#)
- [97] **S. C. Farantos**, and J. Tennyson.  
 Chaos in Molecular Systems? In R. Lefebvre, and S. Mukamel, editors, *Stochasticity and Intramolecular Redistribution of Energy*, pages 15–30. D. Reidel, Dordrecht, 1987. [1](#)
- [98] A. Vegiri, **S. C. Farantos**, P. Papagiannakopoulos, and C. Fotakis.  
 Electronic Deexcitation of  $\text{OH}(A^2\Sigma^+)$  with  $\text{CO}(X^1\Sigma^+)$ ; An Ab Initio Study. In J. C. Whitehead, editor, *Selectivity in Chemical Reactions*, pages 393–402. Kluwer Academic Publishers, 1988. [1](#)
- [99] **S. C. Farantos**, and J. Tennyson.  
 A Ro-Vibrational Study for Regular/Irregular Behaviour of  $\text{CO} - \text{Ar}$  System. In L. S. Cederbaum, A. Amann, and W. Gans, editors, *Fractals Quasicrystals, Chaos, Knots, and Algebraic Quantum Mechanics*, volume 235, pages 195–206. Kluwer Academic Publishers, 1988. [1](#)

- [100] **S. C. Farantos.**  
Classical and Quantum Chaos in Molecular Systems (in Greek). In A. Bountis, and S. Pnevmatikos, editors, *Order and Chaos in Non-Linear Systems*, pages 45–70. Pnevmatikos, 1988. 1
- [101] N. Flytzanis, A. D. Mistriotis, and **S. C. Farantos.**  
Nonlinear Structures in Silicon Clusters.  
*Journal de Physique, Colloque*, 50(3):C3–89–C3–93, 1989. 1
- [102] **S. C. Farantos**, and M. Founargiotakis.  
Study of Molecular Phase Space Structure through Families of Periodic Orbits.  
*NewsLetters in Heavy Particle Dynamics - CCP6*, 12:15–16, 1989. 1
- [103] **S. C. Farantos.**  
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. 1
- [104] **S. C. Farantos.**  
Chemical Dynamics: A Periodic Orbits Approach. In J. Broeckhove and L. Lathouwers, editor, *Time Dependent Quantum Mechanics: Experiments and Theory*, pages 27–43. Plenum Co. Ltd, 1992. 1
- [105] S. Kapetanakis, and **S. C. Farantos.**  
A Classical Mechanical Study of *cis-trans* Isomerization Reaction in  $(\text{H}_2\text{O})_4$  Cluster: An example of non-ergodic behaviour. In S. Xantheas, editor, *Recent Theoretical and Experimental Advances in Hydrogen Bonded Clusters*, volume 561, pages 217–228. Plenum Publishing Corporation., 2000. 1
- [106] **S. C. Farantos.**  
THE\_ELEMENTS: A Beowulf-Class Computer.  
"NewsLetters in SIMU", 1:99, 2000. 1
- [107] **Stavros C. Farantos**, Stamatis Stamatiadis, Nello Nellari, and Djordje Maric.  
ENACTS/Grid Enabling Technologies. <http://www.epcc.ed.ac.uk/enacts/>, Report:1–70, 2002. 1
- [108] M. Joyeux, S. Yu. Grebenschikov, 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". *Adv. Chem. Phys.*, 130:267–303, 2005. 1
- [109] Shi Ying Lin, Hua Guo, and **S. C. Farantos.**  
Resonance States of  $\text{CH}_2(\bar{a}^1A_1)$  and Their Roles in Unimolecular and Bimolecular Reactions.  
*J. Chem. Phys.*, 122(12):124308, 2005. 1

- [110] **S. C. Farantos**, Z.W. Qu, H. Zhu, and R. Schinke,.  
Reactions Paths and elementary bifurcations tracks: the diabatic  $^1B_2$ -state of ozone.  
*Int. J. Bifurcation Chaos Appl. Sci. Eng.*, 16(7):1913–1928, 2006. [1](#)
- [111] 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. [1](#)
- [112] Andreas Mavrandonakis, **Stavros C. Farantos**, and George E. Froudakis.  
Theoretical Modelling of the Glycine Radical Addition to Carbon Nanotubes. *Rev.Adv.Mater.Sci.*, 11:88–91, 2006. [1](#)
- [113] **S. C. Farantos**.  
Periodic Orbits in Biological Molecules: Phase Space Structures and Selectivity in Alanine Dipeptide.  
*J. Chem. Phys.*, 126(17):175101–175107, 2007. [1](#)
- [114] **S. C. Farantos**.  
Periodic Orbits in Biological Molecules: Phase Space Structures and Selectivity in Alanine Dipeptide. *JCP : BioChemical Physics*, 1:issue 5, 2007. [1](#)
- [115] Chuanxiu Xu, Bin Jiang, Daiqian Xie, **Stavros C. Farantos**, Shi Ying Lin, and Hua Guo.  
Analysis of the HO<sub>2</sub> Vibrational Spectrum on an Accurate Ab Initio Potential Energy Surface.  
*J. Phys. Chem. A*, 111(41):10353–10361, 2007. [1](#)
- [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. [1](#)
- [117] A. Mavrandonakis, **S. C. Farantos**, and G. Froudakis.  
Analytical Potential Functions Based on Force-Fields for Studying the Dynamics of Vibrationally Excited and Reactive Carbon Nanotubes Interacting with Aminoacids. *J. Comput. and Theor. Nanosci.*, 6(4):880–885, 2009. [1](#)
- [118] **Stavros C. Farantos**, Reinhard Schinke, Hua Guo, and Marc Joyeux.  
Energy Localization in Molecules, Bifurcation Phenomena, and their Spectroscopic Signatures: The Global View. *Chem. Rev.*, 109(9):4248–4271, 2009. [1](#)
- [119] Jaime Suarez, **Stavros C. Farantos**, Stamatia Stamatiadis, and Lucas Lathouwers.

- A method for solving the molecular Schrödinger Equation in Cartesian coordinates via angular momentum projection operators.  
*Comp. Phys. Comm.*, 180:2025–2033, 2009. [1](#)
- [120] Massimiliano Porrini, Vangelis Daskalakis, **S. C. Farantos**, and Constantinos Varotsis.  
Heme Cavity Dynamics of Photodissociated CO from *ba*<sub>3</sub>-Cytochrome *c* Oxidase: the Role of Ring-D Propionate.  
*J. Phys. Chem. B*, 113(35):12129–12135, 2009. [1](#)
- [121] Vangelis Daskalakis, **Stavros C. Farantos**, Victor Guallar and Constantinos Varotsis.  
Vibrational Resonances and Cu<sub>B</sub> displacement controlled by proton motion in Cytochrome *c* Oxidase.  
*J. Phys. Chem. B*, 114(2):1136–1143, 2010. [1](#)
- [122] Frederic Mauguier, Vladimir Tyuterev, and **Stavros C. Farantos**.  
Bifurcation effects and patterns in the vibrational excited states of isotopically substituted water.  
*Chem. Phys. Letters*, 494:163–169, 2010. [1](#)
- [123] Frederic Mauguier, Michael Rey, Vladimir Tyuterev, Jaime Suarez, and **Stavros C. Farantos**.  
A periodic orbit bifurcation analysis of vibrationally excited isotopologues of sulfur dioxide and water molecules: symmetry breaking substitutions.  
*J. Phys. Chem. A*, 114:9836–9847, 2010. [1](#)
- [124] R. Schinke, J. Suarez, and **S. C. Farantos**.  
Photodissociation of N<sub>2</sub>O: Frustrated NN bond breaking causes diffuse vibrational structures.  
*J. Chem. Phys.*, 133:091103:1–4, 2010. [1](#)
- [125] S. Stamatiadis, and **S. C. Farantos**.  
AUTO\_DERIV: Tool for automatic differentiation of a Fortran code (New Version).  
*Comp. Phys. Comm.*, 181(10):1818–1819, 2010. [1](#)
- [126] Vangelis Daskalakis, **Stavros C. Farantos**, Victor Guallar and Constantinos Varotsis.  
Regulation of electron and proton transfer by the protein matrix of cytochrome *c* oxidase.  
*J. Phys. Chem. B*, 115(13):3648–3655, 2011. [1](#)
- [127] Frederic Mauguier, **Stavros C. Farantos**, Jaime Suarez, and Reinhard Schinke.  
Non-linear dynamics of the photodissociation of nitrous oxide: Equilibrium points, periodic orbits, and transition states.  
*J. Chem. Phys.*, 134(24):244302–12, 2011. [1](#)

- [128] A. Kampanarakis, **S. C. Farantos**, V. Daskalakis and C. Varotsis. Non-Linear Vibrational Modes in Biomolecules: a periodic orbits description. *Chem. Phys.*, 399:258–263, 2012. 1
- [129] M. Porrini, V. Daskalakis, and **S. C. Farantos**. Thermodynamic Perturbation Calculations on Cytochrome *c* Oxidases interacting with small ligands. *RSC Adv.*, 2:5828–5836, 2012. 1
- [130] **Stavros C. Farantos**. ENACTS/Dissemination. <http://www.epcc.ed.ac.uk/enacts/>, Report:1–60, 2005. 2
- [131] **S. C. Farantos**, S. Stamatiadis, L. Lathouwers, and R. Guantes. Grid Enabled Molecular Dynamics: classical and quantum algorithms. In G. Maroulis, Th. Simos, editor, *Lecture Series on Computer and Computational Sciences: Trends and Perspectives in Modern Computational Science*, volume 3, pages 35–50. VSP, 2005. 2
- [132] **S. C. Farantos**. Periodic Orbits in Biological Molecules: Phase Space Structures and Selectivity. In G. Maroulis, Th. Simos, editor, *Lecture Series on Computer and Computational Sciences: Trends and Perspectives in Modern Computational Science*, volume 6, pages 350–356. VSP, 2006. 2
- [133] **Stavros C. Farantos**. Non-Linear Vibrational Normal Modes of Biomolecules. *CPS-IEEE Computer Society*, pages 444–450, 2007. 2
- [134] Vangelis Daskalakis, **Stavros C. Farantos**, and Constantinos Varotsis. Protein dynamics and spectroscopy for ferryl intermediate of Cytochrome *c* Oxidase: A molecular dynamics approach. *AIP Conf. Proc.*, 963-V2A:31–34, 2007. 2
- [135] Jaime Suarez, Stamatis Stamatiadis, **Stavros C. Farantos**, and Lucas Lathouwers. A parallel code for solving the molecular Time Dependent Schrödinger Equation in cartesian coordinates. *AIP Conf. Proc.*, 1148:241–245, 2009. 2
- [136] V. Daskalakis, M. Giatromanolakis, M. Porrini, **S. C. Farantos**, and O. Gervasi. *Computer Physics*, volume ISBN: 978-1-61324-790-7, chapter 4: Grid Computing Multiple Shooting Algorithms for Extended Phase Space Sampling and Long Time Propagation in Molecular Dynamics, pages 297–314. *Nova Science Publishing Co.*, 2012. 2



- [137] V. Daskalakis, **S. C. Farantos** and C. Varotsis.  
Tuning heme functionality: the cases of Cytochrome c Oxidase and Myoglobin Oxidation. *LNCS - Springer-Verlag Berlin, Heidelberg*, ISBN: 978-3-642-31124-6:304-315, 2012. [2](#)
- [138] J. N. Murrell, S. Carter, **S. C. Farantos**, P. Huxley, and A. J. C. Varandas. *Molecular Potential Energy Functions*. John Wiley and Sons Ltd, 1984. [2](#)
- [139] J. N. Murrell, S. F. Kettle, and J. M. Tedder.  
*The Chemical Bond, 2nd Edition*. Crete University Press, 1992. [2](#)
- [140] P. W. Atkins.  
*Physical Chemistry, Part 1*. Crete University Press, 1998. [2](#)

Institutes. Cperi. Iti.Â Multidisciplinary research for regional development and quality of life. CERTH. At a glance. Mission. Organisational Structure. Distinctions. International Collaborations. Contact. Location. INSTITUTES.Â Dr. D. Dimitrakis, chemical engineer - affiliated researcher at CPERI/CERTH talks about solar fuel technology and solar energy utilization applications being investigated in the team he is involved. more. Strengthening proactive cyber defence in the European Union. CERTH participates in the ECHO project (European network of Cybersecurity centres and competence Hub for innovation and Operations), one of four Pilot projects, launched by the European Commission, to establish and operate a Cybersecurity Competence Network. more. In 1986 Skinakas Observatory, jointly supported by RCC, the University of Crete and the Max Planck Institute for Extraterrestrial Physics (Germany) also commenced its operations. In 1987 with the agreement of Prof. George Papatheodorou and Prof.Â Institute of Electronic Structure and Laser - IESL. Institute of Mediterranean Studies - IMS. Institute of Molecular Biology & Biotechnology - IMBB. Biomedical Research Division - BRD (formerly an independent institute, now part of IMBB). Institute of Petroleum Research - IPR. From 1987 to 2000, the Chemical Process Engineering Research Institute (CPERI) based in Thessaloniki was also part of FORTH. Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, Greece. Address: Greece, 71110, Heraklion. Phone: +30 (2810) 39 13 00. Fax: +30 (2810) 39 13 05.