

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. Texeira-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. Founariotakis, **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(A²Σ⁺)* 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. Founariotakis, **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. Founariotakis, 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. Founariotakis. 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. Prosmiti, **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. Prosmiti, and **S. C. Farantos.**
Periodic Orbits, Bifurcation Diagrams and the Spectroscopy of C_2H_2 System.
J. Chem. Phys., 103(9):3299–3314, 1995. [1](#)
- [54] R. Prosmiti, **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 $Mg^{m+}Ar_n$, $m = 1, 2$; $n = 1 - 18$ 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^+Ar_n case.
J. Comput. Chem., 18:1011–1022, 1997. [1](#)
- [59] G. S. Fanourgakis, **S. C. Farantos**, P. Parneix, and Ph. Bréchignac.
An Effective Transition State for a Complex Cluster Isomerization Process: comparison between anharmonic and harmonic models for Mg^+Ar_{12} .
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_2 .
Chem. Phys. Letters, 277:456–464, 1997. [1](#)
- [61] Ch. Beck, Hans-Martin Keller, S. Yu. Grebenschchikov, 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. 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(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. Grebenschchikov, 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. Velegrakis, and S. S. Xantheas. Photofragmentation Spectra and Structures of Sr^+Ar_n , $n = 2–8$ Clusters: Experiment and Theory.
J. Chem. Phys., 109(1):108–120, 1998. [1](#)
- [66] M. Velegrakis, G. E. Froudakis, and **S. C. Farantos**. Stability and Structure of Ni^+Ar_n and Pt^+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 C^+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 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. Velegrakis, and S. S. Xantheas. Photofragmentation Spectra and Potential Energy Surfaces of Sr^+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. Prosmiti, **S. C. Farantos**, and H. Guo. Assigning the Transition from Normal to Local Vibrational Mode in SO₂ by Periodic Orbit. *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 Mechanism of Ar₃. *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. Prosmiti, 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 HeH₂⁺ 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⁺Ne_n, Li⁺Ar_n and Li⁺Kr_n 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 mechanical, 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. Prosmiti, 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. Velegrakis.
Mass Spectra and Structures of Cu⁺Rg_n Clusters (Rg = Ne, 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. Velegrakis.
Photofragmentation Spectra of Sr⁺CO Complex: experiment and ab initio calculations.
Chem. Phys. Letters, 366:231–237, 2002. [1](#)

- [90] R. Prosmiti, 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. Velegrakis.
The Excited States of Sr⁺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 CH₂(\bar{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 OH($A^2\Sigma^+$) with 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 CO – 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. Xanthreas, 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 $\text{CH}_2(\tilde{\alpha}^1\text{A}_1)$ 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 HO₂ 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**, Stamatis 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 *ba₃*-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_B displacement controlled by proton motion in Cytochrome *c* Oxidase.
J. Phys. Chem. B, 114(2):1136–1143, 2010. [1](#)
- [122] Frederic Mauguere, 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 Mauguere, 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 N₂O: 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 Mauguere, **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](#)