Stavros C Farantos

List of Publications by Year
in descending order

120	2,774	159358	233125
papers	citations	30 h-index	45 g-index

123	123	123	1179
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hamiltonian chemical kinetics for studying roaming in formaldehyde dissociation: Linear and nonlinear models. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	0
2	Hamiltonian classical thermodynamics and chemical kinetics. Physica D: Nonlinear Phenomena, 2021, 417, 132813.	1.3	4
3	Hamiltonian thermodynamics in the extended phase space: a unifying theory for non-linear molecular dynamics and classical thermodynamics. Journal of Mathematical Chemistry, 2020, 58, 1247-1280.	0.7	2
4	Dynamics on the Double Morse Potential: A Paradigm for Roaming Reactions with no Saddle Points. Regular and Chaotic Dynamics, 2018, 23, 60-79.	0.3	8
5	Hamiltonian flow over saddles for exploring molecular phase space structures. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170148.	1.6	3
6	Empirical Classification of Trajectory Data: An Opportunity for the Use of Machine Learning in Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 3230-3241.	1.2	16
7	Exit-channel recoil resonances by imaging the photodissociation of single quantum-state-selected OCS molecules. Physical Review A, 2018, 98, .	1.0	5
8	Roaming: A Phase Space Perspective. Annual Review of Physical Chemistry, 2017, 68, 499-524.	4.8	48
9	Recoil Inversion in the Photodissociation of Carbonyl Sulfide near 234Ânm. Physical Review Letters, 2017, 118, 253001.	2.9	11
10	State-specific tunneling lifetimes from classical trajectories: H-atom dissociation in electronically excited pyrrole. Journal of Chemical Physics, 2016, 144, 104105.	1.2	11
11	Phase space barriers and dividing surfaces in the absence of critical points of the potential energy: Application to roaming in ozone. Journal of Chemical Physics, 2016, 144, 054107.	1.2	22
12	Toward Understanding the Roaming Mechanism in H + MgH â† Mg + HH Reaction. Journal of Physical Chemistry A, 2016, 120, 5145-5154.	1.1	24
13	Phase Space Structures Explain Hydrogen Atom Roaming in Formaldehyde Decomposition. Journal of Physical Chemistry Letters, 2015, 6, 4123-4128.	2.1	32
14	Nonlinear Hamiltonian Mechanics Applied to Molecular Dynamics. Springer Briefs in Molecular Science, 2014, , .	0.1	11
15	Roaming dynamics in ion-molecule reactions: Phase space reaction pathways and geometrical interpretation. Journal of Chemical Physics, 2014, 140, 134112.	1.2	35
16	Roaming dynamics in ketene isomerization. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	20
17	Multiple transition states and roaming in ionâ€“molecule reactions: A phase space perspective. Chemical Physics Letters, 2014, 592, 282-287.	1.2	42
18	Quantum and Semiclassical Molecular Dynamics. Springer Briefs in Molecular Science, 2014, , 55-77.	0.1	0

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19	Exploring the topography of free energy surfaces and kinetics of cytochrome c oxidases interacting with small ligands. RSC Advances, 2012, 2, 5828.	1.7	6
20	Non-linear vibrational modes in biomolecules: A periodic orbits description. Chemical Physics, 2012, 399, 258-263.	0.9	3
21	Tuning Heme Functionality: The Cases of Cytochrome c Oxidase and Myoglobin Oxidation. Lecture Notes in Computer Science, 2012, , 304-315.	1.0	0
22	Regulation of Electron and Proton Transfer by the Protein Matrix of CytochromecOxidase. Journal of Physical Chemistry B, 2011, 115, 3648-3655.	1.2	20
23	Non-linear dynamics of the photodissociation of nitrous oxide: Equilibrium points, periodic orbits, and transition states. Journal of Chemical Physics, 2011, 134, 244302.	1.2	13
24	auto_deriv: Tool for automatic differentiation of a Fortran code. Computer Physics Communications, 2010, 181, 1818-1819.	3.0	9
25	Bifurcation effects and patterns in the vibrational excited states of isotopically substituted water. Chemical Physics Letters, 2010, 494, 163-169.	1.2	8
26	A Periodic Orbit Bifurcation Analysis of Vibrationally Excited Isotopologues of Sulfur Dioxide and Water Molecules: Symmetry Breaking Substitutions. Journal of Physical Chemistry A, 2010, 114, 9836-9847.	1.1	12
27	Vibrational Resonances and CuB Displacement Controlled by Proton Motion in Cytochrome c Oxidase. Journal of Physical Chemistry B, 2010, 114, 1136-1143.	1.2	9
28	A method for solving the molecular SchrÃ¶dinger equation in Cartesian coordinates via angular momentum projection operators. Computer Physics Communications, 2009, 180, 2025-2033.	3.0	27
29	Energy Localization in Molecules, Bifurcation Phenomena, and Their Spectroscopic Signatures: The Global View. Chemical Reviews, 2009, 109, 4248-4271.	23.0	72
30	Heme Cavity Dynamics of Photodissociated CO from ba3-Cytochrome c Oxidase: The Role of Ring-D Propionate. Journal of Physical Chemistry B, 2009, 113, 12129-12135.	1.2	7
31	Assigning Vibrational Spectra of Ferryl-Oxo Intermediates of CytochromecOxidase by Periodic Orbits and Molecular Dynamics. Journal of the American Chemical Society, 2008, 130, 12385-12393.	6.6	19
32	Periodic orbits in biological molecules: Phase space structures and selectivity in alanine dipeptide. Journal of Chemical Physics, 2007, 126, 175101.	1.2	16
33	Non-Linear Vibrational Normal Modes of Biomolecules. , 2007, , .		1
34	Analysis of the HO2Vibrational Spectrum on an Accurate Ab Initio Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2007, 111, 10353-10361.	1.1	39
35	Protein Dynamics and Spectroscopy for Ferryl Intermediate of Cytochrome c Oxidase: A Molecular Dynamics Approach. AIP Conference Proceedings, 2007, , .	0.3	0
36	Glycine Interaction with Carbon Nanotubes:Â An ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 6048-6050.	1.2	38

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37	REACTION PATHS AND ELEMENTARY BIFURCATIONS TRACKS: THE DIABATIC 1B2-STATE OF OZONE. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 2006, 16, 1913-1928.	0.7	15
38	Intramolecular Dynamics Along Isomerization and Dissociation Pathways. Advances in Chemical Physics, 2005, , 267-303.	0.3	25
39	Resonances of CH2(aÌƒA11) and their roles in unimolecular and bimolecular reactions. Journal of Chemical Physics, 2005, 122, 124308.	1.2	15
40	The Huggins band of ozone: Unambiguous electronic and vibrational assignment. Journal of Chemical Physics, 2004, 120, 6811-6814.	1.2	24
41	The Huggins band of ozone: A theoretical analysis. Journal of Chemical Physics, 2004, 121, 11731-11745.	1.2	32
42	A regular isomerization path among chaotic vibrational states of <mml:math altimg="si2.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/co	1.2	9
43	The excited states of Sr+CO: photofragmentation spectra and ab initio calculations. Chemical Physics Letters, 2003, 379, 242-247.	1.2	3
44	Periodic orbits and bifurcation diagrams of acetylene/vinylidene revisited. Journal of Chemical Physics, 2003, 118, 8275-8280.	1.2	18
45	The bound state spectrum of HOBr up to the dissociation limit: Evolution of saddle-node bifurcations. Journal of Chemical Physics, 2003, 118, 9643-9652.	1.2	14
46	The vibrational energies of ozone up to the dissociation threshold: Dynamics calculations on an accurate potential energy surface. Journal of Chemical Physics, 2002, 116, 9749-9767.	1.2	166
47	Highly Excited Motion in Molecules:â€‰ Saddle-Node Bifurcations and Their Fingerprints in Vibrational Spectra. Journal of Physical Chemistry A, 2002, 106, 5407-5421.	1.1	82
48	Mass spectra and structures of Cu+Rgn clusters (Rg=Ne, Ar). Chemical Physics, 2002, 280, 43-51.	0.9	23
49	Photofragmentation spectra of Sr+CO complex: experiment and ab initio calculations. Chemical Physics Letters, 2002, 366, 231-237.	1.2	6
50	Response to â€œComment on â€˜High order finite difference algorithms for solving the SchrÃ¶dinger equation in molecular dynamicsâ€™â€‰â€•[J. Chem. Phys. 115, 6794 (2001)]. Journal of Chemical Physics, 2001, 115, 6796-6797.	1.2	0
51	Application of the Characteristic Bisection Method for locating and computing periodic orbits in molecular systems. Computer Physics Communications, 2001, 138, 53-68.	3.0	18
52	Saddle-node states in the spectra of HCO and DCO: a periodic orbit classification of vibrational levels. Chemical Physics Letters, 2001, 344, 565-572.	1.2	9
53	auto_deriv: Tool for automatic differentiation of a fortran code. Computer Physics Communications, 2000, 127, 343-355.	3.0	26
54	Mass spectra and theoretical modeling of Li+Nen, Li+Arn and Li+Krn clusters. Chemical Physics, 2000, 258, 13-20.	0.9	27

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55	Cluster collisions of water tetramers: a classical dynamical study. Chemical Physics, 2000, 262, 337-347.	0.9	0
56	High order finite difference algorithms for solving the SchrÃ¶dinger equation in molecular dynamics. II. Periodic variables. Journal of Chemical Physics, 2000, 113, 10429-10437.	1.2	23
57	Saddle-node bifurcations in the spectrum of HOCl. Journal of Chemical Physics, 2000, 112, 77-93.	1.2	49
58	The vibrational spectrum of deuterated phosphaethyne: A quantum mechanical, classical, and semiclassical analysis. Journal of Chemical Physics, 2000, 112, 8855-8865.	1.2	14
59	High order finite difference algorithms for solving the SchrÃ¶dinger equation in molecular dynamics. Journal of Chemical Physics, 1999, 111, 10827-10835.	1.2	39
60	Coordination of Ti cation embedded in argon clusters. Chemical Physics Letters, 1999, 302, 595-601.	1.2	10
61	Assigning the transition from normal to local vibrational mode in SO2 by periodic orbits. Chemical Physics Letters, 1999, 311, 241-247.	1.2	19
62	HCP CPH ISOMERIZATION: Caught in the Act. Annual Review of Physical Chemistry, 1999, 50, 443-484.	4.8	117
63	Periodic orbitâ€“Quantum mechanical investigation of the inversion mechanism of Ar3. Journal of Chemical Physics, 1999, 111, 10836-10842.	1.2	10
64	Exploring molecular motions in collinear HeH2+ and its isotopic variants using periodic orbits. Physical Chemistry Chemical Physics, 1999, 1, 1105-1113.	1.3	10
65	POMULT: A program for computing periodic orbits in hamiltonian systems based on multiple shooting algorithms. Computer Physics Communications, 1998, 108, 240-258.	3.0	53
66	Binding energies and structures of C+Arn (n=1â€“5), clusters from first principles. Chemical Physics Letters, 1998, 294, 109-116.	1.2	10
67	Periodic orbits and vibrational wave functions for DCP: nonlinear resonances in isotopically substituted molecules. Theoretical Chemistry Accounts, 1998, 100, 147-153.	0.5	3
68	Photofragmentation spectra and structures of Sr+Arn,â€‰n=2â€“8 clusters: Experiment and theory. Journal of Chemical Physics, 1998, 109, 108-120.	1.2	39
69	Stability and structure of Ni+Arn and Pt+Arn clusters. Journal of Chemical Physics, 1998, 109, 4687-4688.	1.2	21
70	Spectroscopic constants of the Xâ€‰2Î£+ and Aâ€‰2Î states of Sr+Ar from first principles: Comparison with experiment. Journal of Chemical Physics, 1998, 108, 46-49.	1.2	19
71	An effective transition state for a complex cluster isomerization process: Comparison between anharmonic and harmonic models for Mg+Ar12. Journal of Chemical Physics, 1997, 106, 4954-4962.	1.2	17
72	Highly excited vibrational states of HCP and their analysis in terms of periodic orbits: The genesis of saddle-node states and their spectroscopic signature. Journal of Chemical Physics, 1997, 107, 9818-9834.	1.2	38

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73	Bifurcation diagrams of periodic orbits for unbound molecular systems: FH2. Chemical Physics Letters, 1997, 277, 456-464.	1.2	16
74	A periodic orbit analysis of the vibrationally highly excited LiNC/LiCN: A comparison with quantum mechanics. Journal of Chemical Physics, 1996, 104, 2921-2931.	1.2	36
75	Normal mode and isomerization bending states in HCP: Periodic orbit assignment and spectroscopic signature. Journal of Chemical Physics, 1996, 104, 10055-10058.	1.2	35
76	Exploring molecular vibrational motions with periodic orbits. International Reviews in Physical Chemistry, 1996, 15, 345-374.	0.9	54
77	Methods for locating periodic orbits in highly unstable systems. Computational and Theoretical Chemistry, 1995, 341, 91-100.	1.5	29
78	Periodic orbits, bifurcation diagrams and the spectroscopy of C2H2 system. Journal of Chemical Physics, 1995, 103, 3299-3314.	1.2	48
79	A periodic orbit approach to the spectroscopy and dynamics of SO2:[Ctilde]1B2 â†' [Xtilde]1A1. Molecular Physics, 1994, 82, 1213-1232.	0.8	17
80	Complex unstable periodic orbits and their manifestation in classical and quantum dynamics. Physical Review E, 1994, 50, 4399-4403.	0.8	19
81	Water clusters: the (H2O)64 case. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1994, 31, 213-217.	1.0	7
82	Water clusters â€" a speculation. Chemical Physics Letters, 1994, 219, 247-251.	1.2	21
83	Classical dynamics of hydrogen bonded systems: Water clusters. Journal of Chemical Physics, 1993, 98, 4059-4075.	1.2	81
84	Periodic Orbits as a Probe to Reveal Exotic States in Vibrationally Excited Molecules: The Saddle-Node States. Laser Chemistry, 1993, 13, 87-99.	0.5	20
85	The importance of periodic orbits in analysing photodissociation resonances: the O3 case. Chemical Physics, 1992, 159, 329-338.	0.9	24
86	Chemical Dynamics: A Periodic Orbits Approach. NATO ASI Series Series B: Physics, 1992, , 27-43.	0.2	5
87	Spectroscopy and Dynamics of Vibrationally Excited Molecules: A Phase Space Structure Analysis. NATO ASI Series Series B: Physics, 1992, , 301-316.	0.2	0
88	Periodic orbits and quantum localization in the van der Waals system COî—¸Ar. Chemical Physics, 1991, 154, 55-62.	0.9	10
89	On the consistency between recent experimental results and a previous theoretical analysis for HCN. Journal of Chemical Physics, 1991, 94, 2376-2376.	1.2	5
90	The photodissociation of O3: A classical dynamical approach for the interpretation of the recurrences in the autocorrelation function. Journal of Chemical Physics, 1991, 94, 4887-4895.	1.2	19

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91	A classical dynamical investigation of the mechanism of electronic quenching of OH(A2Î£+) in collisions with CO(X1Î£+). Molecular Physics, 1990, 69, 129-146.	0.8	9
92	The extraction of dynamics from spectra in regions of mixed chaotic and regular motion: The HCN case. Chemical Physics Letters, 1990, 166, 71-76.	1.2	13
93	Ab initio potential energy surfaces for studying the quenching of CH(A 2Î") by H2(X 1Î£g+). Chemical Physics Letters, 1990, 167, 278-284.	1.2	11
94	Wave packet dynamics and phase space structure of HCN molecule. Chemical Physics, 1990, 142, 345-359.	0.9	23
95	The extraction of dynamics and the classical mechanical simulation of low resolution regular and chaotic spectra: HCN/HNC. Journal of Chemical Physics, 1990, 93, 76-86.	1.2	32
96	Potential model for silicon clusters. Physical Review B, 1989, 39, 1212-1218.	1.1	61
97	Periodic orbits, bifurcations, and quantum mechanical eigenfunctions and spectra. Journal of Chemical Physics, 1989, 91, 1389-1402.	1.2	47
98	Study of molecular phase space structure through families of periodic orbits. Chemical Physics, 1989, 135, 347-356.	0.9	18
99	Regular/irregular phase space structure of HCN/HNC. Journal of Chemical Physics, 1988, 88, 1598-1607.	1.2	37
100	A Ro-Vibrational Study of Regular/Irregular Behaviour of the CO-Ar System. , 1988, , 195-206.		1
101	Chaos in Molecular Systems?. , 1987, , 15-30.		7
102	Transition intensities and fluorescence lifetimes for regular and chaotic states of LiCN. Chemical Physics, 1986, 104, 399-407.	0.9	17
103	On the vibrational Bornâ€"Oppenheimer separation scheme for molecules with regular and chaotic states. Journal of Chemical Physics, 1986, 84, 6210-6217.	1.2	24
104	Chaotic structure in the phase space of acetylene. Journal of Chemical Physics, 1986, 85, 641-642.	1.2	20
105	A classical trajectory study of the reaction He(1S) + H2(B1Î£u+) â†' HeH(A2Î£+) + H(2S). Molecular Physics, 1986, 59, 1273-1275.	0.8	3
106	A quasiclassical study of collisions of He with HD(B1Î£+u). Molecular Physics, 1985, 54, 835-845.	0.8	13
107	Routes to vibrational chaos in triatomic molecules. Chemical Physics, 1985, 93, 237-244.	0.9	35
108	Rovibrational spectrum of the excited potential energy surface of He+H2 (Bâ€‰1Î£u+). Journal of Chemical Physics, 1985, 82, 2163-2164.	1.2	8

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109	Quantum and classical vibrational chaos in floppy molecules. Journal of Chemical Physics, 1985, 82, 800-809.	1.2	63
110	Analytical ab initio potential-energy surfaces for the ground and the first singlet excited states of HeH2. Chemical Physics Letters, 1984, 108, 367-372.	1.2	19
111	A non-van der Waals minimum of the He(1S) + H2(B 1Î£u+) excited surface. Chemical Physics Letters, 1983, 100, 263-267.	1.2	38
112	Exponentially divergent trajectories and RRKM behaviour of Ar3 clusters. Chemical Physics Letters, 1982, 92, 379-382.	1.2	13
113	Monte Carlo calculations of classical density of states for non-separable polyatomic potential energy surfaces. Chemical Physics, 1982, 68, 109-117.	0.9	30
114	Evaluation of an upper bound of the maximal lyapunov characteristic number by Monte Carlo integration in the chaotic regions of phase space. Chemical Physics, 1982, 71, 157-160.	0.9	3
115	Studies on atomâ€“triatom reactive scattering. Classical dynamics of H + C2H collisions. Journal of the Chemical Society, Faraday Transactions 2, 1981, 77, 2279-2288.	1.1	1
116	On the transition from quasiperiodic to stochastic classical motion on real polyatomic potential energy surfaces. Chemical Physics, 1981, 55, 205-214.	0.9	46
117	A classical trajectory study of the reaction H + HCOâ†'H2+ CO. Molecular Physics, 1980, 40, 883-891.	0.8	16
118	Classical dynamics of the O + ClO ? Cl + O2 and Cl + O3 ? ClO + O2 reactions. International Journal of Quantum Chemistry, 1978, 14, 659-674.	1.0	39
119	An analytical function for the potential energy surface of ozone. Molecular Physics, 1977, 34, 1185-1188.	0.8	26
120	Analytical potentials for triatomic molecules from spectroscopic data. Molecular Physics, 1977, 34, 947-962.	0.8	59