

Stavros C Farantos

List of Publications by Year in descending order

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120
papers

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citations

159358

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45
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123
all docs

123
docs citations

123
times ranked

1179
citing authors

#	ARTICLE	IF	CITATIONS
1	The vibrational energies of ozone up to the dissociation threshold: Dynamics calculations on an accurate potential energy surface. <i>Journal of Chemical Physics</i> , 2002, 116, 9749-9767.	1.2	166
2	HCP CPH ISOMERIZATION: Caught in the Act. <i>Annual Review of Physical Chemistry</i> , 1999, 50, 443-484.	4.8	117
3	Highly Excited Motion in Molecules: Saddle-Node Bifurcations and Their Fingerprints in Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2002, 106, 5407-5421.	1.1	82
4	Classical dynamics of hydrogen bonded systems: Water clusters. <i>Journal of Chemical Physics</i> , 1993, 98, 4059-4075.	1.2	81
5	Energy Localization in Molecules, Bifurcation Phenomena, and Their Spectroscopic Signatures: The Global View. <i>Chemical Reviews</i> , 2009, 109, 4248-4271.	23.0	72
6	Quantum and classical vibrational chaos in floppy molecules. <i>Journal of Chemical Physics</i> , 1985, 82, 800-809.	1.2	63
7	Potential model for silicon clusters. <i>Physical Review B</i> , 1989, 39, 1212-1218.	1.1	61
8	Analytical potentials for triatomic molecules from spectroscopic data. <i>Molecular Physics</i> , 1977, 34, 947-962.	0.8	59
9	Exploring molecular vibrational motions with periodic orbits. <i>International Reviews in Physical Chemistry</i> , 1996, 15, 345-374.	0.9	54
10	POMULT: A program for computing periodic orbits in hamiltonian systems based on multiple shooting algorithms. <i>Computer Physics Communications</i> , 1998, 108, 240-258.	3.0	53
11	Saddle-node bifurcations in the spectrum of HOCl. <i>Journal of Chemical Physics</i> , 2000, 112, 77-93.	1.2	49
12	Periodic orbits, bifurcation diagrams and the spectroscopy of C ₂ H ₂ system. <i>Journal of Chemical Physics</i> , 1995, 103, 3299-3314.	1.2	48
13	Roaming: A Phase Space Perspective. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 499-524.	4.8	48
14	Periodic orbits, bifurcations, and quantum mechanical eigenfunctions and spectra. <i>Journal of Chemical Physics</i> , 1989, 91, 1389-1402.	1.2	47
15	On the transition from quasiperiodic to stochastic classical motion on real polyatomic potential energy surfaces. <i>Chemical Physics</i> , 1981, 55, 205-214.	0.9	46
16	Multiple transition states and roaming in ion-molecule reactions: A phase space perspective. <i>Chemical Physics Letters</i> , 2014, 592, 282-287.	1.2	42
17	Classical dynamics of the O + ClO → Cl + O ₂ and Cl + O ₃ → ClO + O ₂ reactions. <i>International Journal of Quantum Chemistry</i> , 1978, 14, 659-674.	1.0	39
18	Photofragmentation spectra and structures of Sr+Ar _n , n=2-8 clusters: Experiment and theory. <i>Journal of Chemical Physics</i> , 1998, 109, 108-120.	1.2	39

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19	High order finite difference algorithms for solving the Schrödinger equation in molecular dynamics. Journal of Chemical Physics, 1999, 111, 10827-10835.	1.2	39
20	Analysis of the HO ₂ Vibrational Spectrum on an Accurate Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2007, 111, 10353-10361.	1.1	39
21	A non-van der Waals minimum of the He(1S) + H ₂ (B Σ^+_{u+}) excited surface. Chemical Physics Letters, 1983, 100, 263-267.	1.2	38
22	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
23	Glycine Interaction with Carbon Nanotubes: An ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 6048-6050.	1.2	38
24	Regular/irregular phase space structure of HCN/HNC. Journal of Chemical Physics, 1988, 88, 1598-1607.	1.2	37
25	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
26	Routes to vibrational chaos in triatomic molecules. Chemical Physics, 1985, 93, 237-244.	0.9	35
27	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
28	Roaming dynamics in ion-molecule reactions: Phase space reaction pathways and geometrical interpretation. Journal of Chemical Physics, 2014, 140, 134112.	1.2	35
29	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
30	The Huggins band of ozone: A theoretical analysis. Journal of Chemical Physics, 2004, 121, 11731-11745.	1.2	32
31	Phase Space Structures Explain Hydrogen Atom Roaming in Formaldehyde Decomposition. Journal of Physical Chemistry Letters, 2015, 6, 4123-4128.	2.1	32
32	Monte Carlo calculations of classical density of states for non-separable polyatomic potential energy surfaces. Chemical Physics, 1982, 68, 109-117.	0.9	30
33	Methods for locating periodic orbits in highly unstable systems. Computational and Theoretical Chemistry, 1995, 341, 91-100.	1.5	29
34	Mass spectra and theoretical modeling of Li+Nen, Li+Arn and Li+Krn clusters. Chemical Physics, 2000, 258, 13-20.	0.9	27
35	A method for solving the molecular Schrödinger equation in Cartesian coordinates via angular momentum projection operators. Computer Physics Communications, 2009, 180, 2025-2033.	3.0	27
36	An analytical function for the potential energy surface of ozone. Molecular Physics, 1977, 34, 1185-1188.	0.8	26

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37	auto_deriv: Tool for automatic differentiation of a fortran code. Computer Physics Communications, 2000, 127, 343-355.	3.0	26
38	Intramolecular Dynamics Along Isomerization and Dissociation Pathways. Advances in Chemical Physics, 2005, , 267-303.	0.3	25
39	On the vibrational Born-Oppenheimer separation scheme for molecules with regular and chaotic states. Journal of Chemical Physics, 1986, 84, 6210-6217.	1.2	24
40	The importance of periodic orbits in analysing photodissociation resonances: the O3 case. Chemical Physics, 1992, 159, 329-338.	0.9	24
41	The Huggins band of ozone: Unambiguous electronic and vibrational assignment. Journal of Chemical Physics, 2004, 120, 6811-6814.	1.2	24
42	Toward Understanding the Roaming Mechanism in H + MgH → Mg + HH Reaction. Journal of Physical Chemistry A, 2016, 120, 5145-5154.	1.1	24
43	Wave packet dynamics and phase space structure of HCN molecule. Chemical Physics, 1990, 142, 345-359.	0.9	23
44	High order finite difference algorithms for solving the Schrödinger equation in molecular dynamics. II. Periodic variables. Journal of Chemical Physics, 2000, 113, 10429-10437.	1.2	23
45	Mass spectra and structures of Cu+Rgn clusters (Rg=Ne, Ar). Chemical Physics, 2002, 280, 43-51.	0.9	23
46	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
47	Water clusters – a speculation. Chemical Physics Letters, 1994, 219, 247-251.	1.2	21
48	Stability and structure of Ni+Arn and Pt+Arn clusters. Journal of Chemical Physics, 1998, 109, 4687-4688.	1.2	21
49	Chaotic structure in the phase space of acetylene. Journal of Chemical Physics, 1986, 85, 641-642.	1.2	20
50	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
51	Regulation of Electron and Proton Transfer by the Protein Matrix of Cytochrome <i>c</i> Oxidase. Journal of Physical Chemistry B, 2011, 115, 3648-3655.	1.2	20
52	Roaming dynamics in ketene isomerization. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	20
53	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
54	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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55	Complex unstable periodic orbits and their manifestation in classical and quantum dynamics. <i>Physical Review E</i> , 1994, 50, 4399-4403.	0.8	19
56	Spectroscopic constants of the $X^{\infty}2^{\infty}+$ and $A^{\infty}2^{\infty}$ states of Sr+Ar from first principles: Comparison with experiment. <i>Journal of Chemical Physics</i> , 1998, 108, 46-49.	1.2	19
57	Assigning the transition from normal to local vibrational mode in SO ₂ by periodic orbits. <i>Chemical Physics Letters</i> , 1999, 311, 241-247.	1.2	19
58	Assigning Vibrational Spectra of Ferryl-Oxo Intermediates of Cytochrome c Oxidase by Periodic Orbits and Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2008, 130, 12385-12393.	6.6	19
59	Study of molecular phase space structure through families of periodic orbits. <i>Chemical Physics</i> , 1989, 135, 347-356.	0.9	18
60	Application of the Characteristic Bisection Method for locating and computing periodic orbits in molecular systems. <i>Computer Physics Communications</i> , 2001, 138, 53-68.	3.0	18
61	Periodic orbits and bifurcation diagrams of acetylene/vinylidene revisited. <i>Journal of Chemical Physics</i> , 2003, 118, 8275-8280.	1.2	18
62	Transition intensities and fluorescence lifetimes for regular and chaotic states of LiCN. <i>Chemical Physics</i> , 1986, 104, 399-407.	0.9	17
63	A periodic orbit approach to the spectroscopy and dynamics of SO ₂ : $1B_2$ \leftrightarrow $1A_1$. <i>Molecular Physics</i> , 1994, 82, 1213-1232.	0.8	17
64	An effective transition state for a complex cluster isomerization process: Comparison between anharmonic and harmonic models for Mg+Ar ₁₂ . <i>Journal of Chemical Physics</i> , 1997, 106, 4954-4962.	1.2	17
65	A classical trajectory study of the reaction H + HCO \rightarrow H ₂ + CO. <i>Molecular Physics</i> , 1980, 40, 883-891.	0.8	16
66	Bifurcation diagrams of periodic orbits for unbound molecular systems: FH ₂ . <i>Chemical Physics Letters</i> , 1997, 277, 456-464.	1.2	16
67	Periodic orbits in biological molecules: Phase space structures and selectivity in alanine dipeptide. <i>Journal of Chemical Physics</i> , 2007, 126, 175101.	1.2	16
68	Empirical Classification of Trajectory Data: An Opportunity for the Use of Machine Learning in Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2018, 122, 3230-3241.	1.2	16
69	Resonances of CH ₂ ($1A_1$) and their roles in unimolecular and bimolecular reactions. <i>Journal of Chemical Physics</i> , 2005, 122, 124308.	1.2	15
70	REACTION PATHS AND ELEMENTARY BIFURCATIONS TRACKS: THE DIABATIC $1B_2$ -STATE OF OZONE. <i>International Journal of Bifurcation and Chaos in Applied Sciences and Engineering</i> , 2006, 16, 1913-1928.	0.7	15
71	The vibrational spectrum of deuterated phosphoethyne: A quantum mechanical, classical, and semiclassical analysis. <i>Journal of Chemical Physics</i> , 2000, 112, 8855-8865.	1.2	14
72	The bound state spectrum of HOBr up to the dissociation limit: Evolution of saddle-node bifurcations. <i>Journal of Chemical Physics</i> , 2003, 118, 9643-9652.	1.2	14

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73	Exponentially divergent trajectories and RRKM behaviour of Ar ₃ clusters. Chemical Physics Letters, 1982, 92, 379-382.	1.2	13
74	A quasiclassical study of collisions of He with HD(B ¹ Σ ⁺ u). Molecular Physics, 1985, 54, 835-845.	0.8	13
75	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
76	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
77	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
78	Ab initio potential energy surfaces for studying the quenching of CH(A ² Π ⁺) by H ₂ (X ¹ Σ ⁺ g ⁺). Chemical Physics Letters, 1990, 167, 278-284.	1.2	11
79	Nonlinear Hamiltonian Mechanics Applied to Molecular Dynamics. Springer Briefs in Molecular Science, 2014, , .	0.1	11
80	State-specific tunneling lifetimes from classical trajectories: H-atom dissociation in electronically excited pyrrole. Journal of Chemical Physics, 2016, 144, 104105.	1.2	11
81	Recoil Inversion in the Photodissociation of Carbonyl Sulfide near 234Ånm. Physical Review Letters, 2017, 118, 253001.	2.9	11
82	Periodic orbits and quantum localization in the van der Waals system CO ⁺ -Ar. Chemical Physics, 1991, 154, 55-62.	0.9	10
83	Binding energies and structures of C+Ar _n (n=1-5), clusters from first principles. Chemical Physics Letters, 1998, 294, 109-116.	1.2	10
84	Coordination of Ti cation embedded in argon clusters. Chemical Physics Letters, 1999, 302, 595-601.	1.2	10
85	Periodic orbit-Quantum mechanical investigation of the inversion mechanism of Ar ₃ . Journal of Chemical Physics, 1999, 111, 10836-10842.	1.2	10
86	Exploring molecular motions in collinear HeH ₂ ⁺ and its isotopic variants using periodic orbits. Physical Chemistry Chemical Physics, 1999, 1, 1105-1113.	1.3	10
87	A classical dynamical investigation of the mechanism of electronic quenching of OH(A ² Σ ⁺) in collisions with CO(X ¹ Σ ⁺). Molecular Physics, 1990, 69, 129-146.	0.8	9
88	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
89	A regular-irregular connection path among chaotic vibrational states of H_2O^+ . $\text{display= "inline" overflow= "scroll" xmlns:xocs= "http://www.elsevier.com/xml/xocs/dtd" xmlns:xs= "http://www.w3.org/2001/XMLSchema" xmlns:xsi= "http://www.w3.org/2001/XMLSchema-instance" xmlns= "http://www.elsevier.com/xml/ja/dtd" xmlns:ja= "http://www.elsevier.com/xml/ja/dtd" xmlns:mml= "http://www.w3.org/1998/Math/MathML" xmlns:tb= "http://www.elsevier.com/xml/common/table/dtd" xmlns:tbl_struct= "http://www.elsevier.com/xml/common/table-struct/dtd" }$	1.2	9
90	auto_deriv: Tool for automatic differentiation of a Fortran code. Computer Physics Communications, 2010, 181, 1818-1819.	3.0	9

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91	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
92	Rovibrational spectrum of the excited potential energy surface of He+H2 (B $\hat{\epsilon}$ 1 $\hat{\xi}$ u+). Journal of Chemical Physics, 1985, 82, 2163-2164.	1.2	8
93	Bifurcation effects and patterns in the vibrational excited states of isotopically substituted water. Chemical Physics Letters, 2010, 494, 163-169.	1.2	8
94	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
95	Water clusters: the (H2O) ₆₄ case. Zeitschrift für Physik D-Atoms Molecules and Clusters, 1994, 31, 213-217.	1.0	7
96	Heme Cavity Dynamics of Photodissociated CO from ba ₃ -Cytochrome c Oxidase: The Role of Ring-D Propionate. Journal of Physical Chemistry B, 2009, 113, 12129-12135.	1.2	7
97	Chaos in Molecular Systems?. , 1987, , 15-30.		7
98	Photofragmentation spectra of Sr+CO complex: experiment and ab initio calculations. Chemical Physics Letters, 2002, 366, 231-237.	1.2	6
99	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
100	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
101	Exit-channel recoil resonances by imaging the photodissociation of single quantum-state-selected OCS molecules. Physical Review A, 2018, 98, .	1.0	5
102	Chemical Dynamics: A Periodic Orbits Approach. NATO ASI Series Series B: Physics, 1992, , 27-43.	0.2	5
103	Hamiltonian classical thermodynamics and chemical kinetics. Physica D: Nonlinear Phenomena, 2021, 417, 132813.	1.3	4
104	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
105	A classical trajectory study of the reaction He(1S) + H2(B1 $\hat{\xi}$ u+) \hat{a} t' HeH(A2 $\hat{\xi}$ +) + H(2S). Molecular Physics, 1986, 59, 1273-1275.	0.8	3
106	Periodic orbits and vibrational wave functions for DCP: nonlinear resonances in isotopically substituted molecules. Theoretical Chemistry Accounts, 1998, 100, 147-153.	0.5	3
107	The excited states of Sr+CO: photofragmentation spectra and ab initio calculations. Chemical Physics Letters, 2003, 379, 242-247.	1.2	3
108	Non-linear vibrational modes in biomolecules: A periodic orbits description. Chemical Physics, 2012, 399, 258-263.	0.9	3

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109	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
110	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
111	Studies on atom-atom reactive scattering. Classical dynamics of H + C2H collisions. Journal of the Chemical Society, Faraday Transactions 2, 1981, 77, 2279-2288.	1.1	1
112	Non-Linear Vibrational Normal Modes of Biomolecules. , 2007, , .		1
113	A Ro-Vibrational Study of Regular/Irregular Behaviour of the CO-Ar System. , 1988, , 195-206.		1
114	Cluster collisions of water tetramers: a classical dynamical study. Chemical Physics, 2000, 262, 337-347.	0.9	0
115	Response to "Comment on "High order finite difference algorithms for solving the Schrödinger equation in molecular dynamics" [J. Chem. Phys. 115, 6794 (2001)]. Journal of Chemical Physics, 2001, 115, 6796-6797.		0
116	Protein Dynamics and Spectroscopy for Ferryl Intermediate of Cytochrome c Oxidase: A Molecular Dynamics Approach. AIP Conference Proceedings, 2007, , .	0.3	0
117	Tuning Heme Functionality: The Cases of Cytochrome c Oxidase and Myoglobin Oxidation. Lecture Notes in Computer Science, 2012, , 304-315.	1.0	0
118	Quantum and Semiclassical Molecular Dynamics. Springer Briefs in Molecular Science, 2014, , 55-77.	0.1	0
119	Spectroscopy and Dynamics of Vibrationally Excited Molecules: A Phase Space Structure Analysis. NATO ASI Series Series B: Physics, 1992, , 301-316.	0.2	0
120	Hamiltonian chemical kinetics for studying roaming in formaldehyde dissociation: Linear and nonlinear models. Journal of Physical Organic Chemistry, 2022, 35, .	0.9	0