

Gregory S Ezra

List of Publications by Year in descending order

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46
papers

1,450
citations

257101

24
h-index

315357

38
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46
all docs

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docs citations

46
times ranked

710
citing authors

#	ARTICLE	IF	CITATIONS
1	Semiclassical quantization using classical perturbation theory: Algebraic quantization of multidimensional systems. <i>Journal of Chemical Physics</i> , 1987, 86, 6270-6282.	1.2	134
2	EBK quantization of nonseparable systems: A Fourier transform method. <i>Journal of Chemical Physics</i> , 1985, 83, 2990-3001.	1.2	126
3	Classical and semiclassical mechanics of strongly resonant systems: A Fourier transform approach. <i>Journal of Chemical Physics</i> , 1987, 86, 279-307.	1.2	118
4	Transport and turnstiles in multidimensional Hamiltonian mappings for unimolecular fragmentation: Application to van der Waals predissociation. <i>Journal of Chemical Physics</i> , 1991, 94, 2648-2668.	1.2	86
5	Microcanonical rates, gap times, and phase space dividing surfaces. <i>Journal of Chemical Physics</i> , 2009, 130, 164118.	1.2	62
6	Eigenstate assignments and the quantum-classical correspondence for highly-excited vibrational states of the Baggot H ₂ O Hamiltonian. <i>Journal of Chemical Physics</i> , 1997, 107, 156-179.	1.2	57
7	Nonstatistical dynamics on potentials exhibiting reaction path bifurcations and valley-ridge inflection points. <i>Journal of Chemical Physics</i> , 2013, 139, 154108.	1.2	48
8	Roaming: A Phase Space Perspective. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 499-524.	4.8	48
9	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
10	Classical, quantum mechanical, and semiclassical representations of resonant dynamics: A unified treatment. <i>Journal of Chemical Physics</i> , 1987, 87, 284-302.	1.2	41
11	Nonstatistical dynamics on the caldera. <i>Journal of Chemical Physics</i> , 2014, 141, 034111.	1.2	38
12	Roaming dynamics in ion-molecule reactions: Phase space reaction pathways and geometrical interpretation. <i>Journal of Chemical Physics</i> , 2014, 140, 134112.	1.2	35
13	On the Statistical Mechanics of Non-Hamiltonian Systems: The Generalized Liouville Equation, Entropy, and Time-Dependent Metrics. <i>Journal of Mathematical Chemistry</i> , 2004, 35, 29-53.	0.7	34
14	Reaction Path Bifurcation in an Electrocyclic Reaction: Ring-Opening of the Cyclopropyl Radical. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6611-6630.	1.1	32
15	Phase Space Structures Explain Hydrogen Atom Roaming in Formaldehyde Decomposition. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4123-4128.	2.1	32
16	Nonadiabatic semiclassical dynamics in the mixed quantum-classical initial value representation. <i>Journal of Chemical Physics</i> , 2018, 148, 102326.	1.2	32
17	Vibrational Echoes: Dephasing, Rephasing, and the Stability of Classical Trajectories. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6536-6543.	1.2	31
18	Periodic orbit analysis of molecular vibrational spectra: Spectral patterns and dynamical bifurcations in Fermi resonant systems. <i>Journal of Chemical Physics</i> , 1996, 104, 26-35.	1.2	30

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19	Optical response functions with semiclassical dynamics. <i>Journal of Chemical Physics</i> , 2003, 119, 1003-1020.	1.2	28
20	Vibrationally induced rotational axis switching: A novel mechanism for vibrational mode coupling. <i>Journal of Chemical Physics</i> , 1992, 97, 5956-5963.	1.2	27
21	Semiclassical quantization of a classical analog for the Jahn-Teller system. <i>Journal of Chemical Physics</i> , 1986, 85, 2089-2098.	1.2	26
22	Sampling Phase Space Dividing Surfaces Constructed from Normally Hyperbolic Invariant Manifolds (NHIMs). <i>Journal of Physical Chemistry A</i> , 2018, 122, 8354-8362.	1.1	26
23	Avoided crossings and resummation of nearly resonant molecular vibrations: Reconstruction of an effective secular equation. <i>Journal of Chemical Physics</i> , 1989, 90, 6378-6390.	1.2	25
24	Reversible measure-preserving integrators for non-Hamiltonian systems. <i>Journal of Chemical Physics</i> , 2006, 125, 034104.	1.2	25
25	Toward Understanding the Roaming Mechanism in $H + MgH \rightarrow Mg + HH$ Reaction. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5145-5154.	1.1	24
26	Phase space barriers and dividing surfaces in the absence of critical points of the potential energy: Application to roaming in ozone. <i>Journal of Chemical Physics</i> , 2016, 144, 054107.	1.2	22
27	Roaming dynamics in ketene isomerization. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	20
28	Vibrational deactivation in Kr/O ₂ +collisions: Role of complex formation and potential anisotropy. <i>Journal of Chemical Physics</i> , 1992, 97, 6322-6334.	1.2	18
29	Isomerization dynamics of a buckled nanobeam. <i>Physical Review E</i> , 2012, 86, 056218.	0.8	18
30	BIFURCATIONS OF NORMALLY HYPERBOLIC INVARIANT MANIFOLDS IN ANALYTICALLY TRACTABLE MODELS AND CONSEQUENCES FOR REACTION DYNAMICS. <i>International Journal of Bifurcation and Chaos in Applied Sciences and Engineering</i> , 2013, 23, 1330043.	0.7	17
31	Periodic orbit analysis of molecular vibrational spectra: 1:1 resonant coupled modes. <i>Journal of Chemical Physics</i> , 1995, 103, 1375-1383.	1.2	16
32	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
33	Intramolecular dynamics and multiresonant absorption spectroscopy. II. Power broadening and superposition states in double resonant two-photon excitation. <i>Journal of Chemical Physics</i> , 1985, 83, 5369-5379.	1.2	15
34	Fragmentation kinetics of a Morse oscillator chain under tension. <i>Chemical Physics</i> , 2007, 337, 11-32.	0.9	14
35	Geometric Approach to Response Theory in Non-Hamiltonian Systems. <i>Journal of Mathematical Chemistry</i> , 2002, 32, 339-360.	0.7	13
36	Impenetrable barriers in phase space for deterministic thermostats. <i>Journal of Physics A: Mathematical and Theoretical</i> , 2009, 42, 042001.	0.7	12

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37	PERTURB: A special-purpose algebraic manipulation program for classical perturbation theory. Journal of Computational Chemistry, 1987, 8, 397-411.	1.5	9
38	Phase space structure and dynamics for the Hamiltonian isokinetic thermostat. Journal of Chemical Physics, 2010, 133, 014105.	1.2	9
39	Bulgac-Kusnezov-Nosé-Hoover thermostats. Physical Review E, 2010, 81, 036705.	0.8	8
40	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
41	Semiclassical IVR approach to rotational excitation of non-polar diatomic molecules by non-resonant laser pulses. Chemical Physics Letters, 2006, 420, 296-303.	1.2	7
42	Roaming at Constant Kinetic Energy: Chesnavich's Model and the Hamiltonian Isokinetic Thermostat. Regular and Chaotic Dynamics, 2019, 24, 615-627.	0.3	6
43	Quantum state reconstruction for rigid rotors. Chemical Physics Letters, 2007, 440, 341-347.	1.2	5
44	Using Lagrangian Descriptors to Uncover Invariant Structures in Chesnavich's Isokinetic Model with Application to Roaming. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 2020, 30, 2050076.	0.7	5
45	The Chesnavich Model for Ion-Molecule Reactions: A Rigid Body Coupled to a Particle. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 2019, 29, 1950025.	0.7	3
46	Isomerization kinetics of a strained Morse oscillator ring. Chemical Physics, 2011, 381, 80-87.	0.9	2