Gregory S Ezra

List of Publications by Year
in descending order

46 papers	1,450 citations	257101 24 h-index	315357 38 g-index
46 all docs	46 docs citations	46 times ranked	710 citing authors

#	Article	IF	Citations
1	Using Lagrangian Descriptors to Uncover Invariant Structures in Chesnavichâ€™s Isokinetic Model with Application to Roaming. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 2020, 30, 2050076.	0.7	5
2	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
3	Roaming at Constant Kinetic Energy: Chesnavichâ€™s Model and the Hamiltonian Isokinetic Thermostat. Regular and Chaotic Dynamics, 2019, 24, 615-627.	0.3	6
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	Nonadiabatic semiclassical dynamics in the mixed quantum-classical initial value representation. Journal of Chemical Physics, 2018, 148, 102326.	1.2	32
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	Sampling Phase Space Dividing Surfaces Constructed from Normally Hyperbolic Invariant Manifolds (NHIMs). Journal of Physical Chemistry A, 2018, 122, 8354-8362.	1.1	26
8	Roaming: A Phase Space Perspective. Annual Review of Physical Chemistry, 2017, 68, 499-524.	4.8	48
9	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
10	Toward Understanding the Roaming Mechanism in H + MgH â†’ Mg + HH Reaction. Journal of Physical Chemistry A, 2016, 120, 5145-5154.	1.1	24
11	Reaction Path Bifurcation in an Electrocyclic Reaction: Ring-Opening of the Cyclopropyl Radical. Journal of Physical Chemistry A, 2015, 119, 6611-6630.	1.1	32
12	Phase Space Structures Explain Hydrogen Atom Roaming in Formaldehyde Decomposition. Journal of Physical Chemistry Letters, 2015, 6, 4123-4128.	2.1	32
13	Nonstatistical dynamics on the caldera. Journal of Chemical Physics, 2014, 141, 034111.	1.2	38
14	Roaming dynamics in ion-molecule reactions: Phase space reaction pathways and geometrical interpretation. Journal of Chemical Physics, 2014, 140, 134112.	1.2	35
15	Roaming dynamics in ketene isomerization. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	20
16	Multiple transition states and roaming in ionâ€“molecule reactions: A phase space perspective. Chemical Physics Letters, 2014, 592, 282-287.	1.2	42
17	Nonstatistical dynamics on potentials exhibiting reaction path bifurcations and valley-ridge inflection points. Journal of Chemical Physics, 2013, 139, 154108.	1.2	48
18	BIFURCATIONS OF NORMALLY HYPERBOLIC INVARIANT MANIFOLDS IN ANALYTICALLY TRACTABLE MODELS AND CONSEQUENCES FOR REACTION DYNAMICS. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 2013, 23, 1330043.	0.7	17

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19	Isomerization dynamics of a buckled nanobeam. Physical Review E, 2012, 86, 056218.	0.8	18
20	Isomerization kinetics of a strained Morse oscillator ring. Chemical Physics, 2011, 381, 80-87.	0.9	2
21	Phase space structure and dynamics for the Hamiltonian isokinetic thermostat. Journal of Chemical Physics, 2010, 133, 014105.	1.2	9
22	Bulgac-Kusnezov-NosÃ©-Hoover thermostats. Physical Review E, 2010, 81, 036705.	0.8	8
23	Microcanonical rates, gap times, and phase space dividing surfaces. Journal of Chemical Physics, 2009, 130, 164118.	1.2	62
24	Impenetrable barriers in phase space for deterministic thermostats. Journal of Physics A: Mathematical and Theoretical, 2009, 42, 042001.	0.7	12
25	Quantum state reconstruction for rigid rotors. Chemical Physics Letters, 2007, 440, 341-347.	1.2	5
26	Fragmentation kinetics of a Morse oscillator chain under tension. Chemical Physics, 2007, 337, 11-32.	0.9	14
27	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
28	Reversible measure-preserving integrators for non-Hamiltonian systems. Journal of Chemical Physics, 2006, 125, 034104.	1.2	25
29	On the Statistical Mechanics of Non-Hamiltonian Systems: The Generalized Liouville Equation, Entropy, and Time-Dependent Metrics. Journal of Mathematical Chemistry, 2004, 35, 29-53.	0.7	34
30	Vibrational Echoes:â€‰ Dephasing, Rephasing, and the Stability of Classical Trajectories. Journal of Physical Chemistry B, 2004, 108, 6536-6543.	1.2	31
31	Optical response functions with semiclassical dynamics. Journal of Chemical Physics, 2003, 119, 1003-1020.	1.2	28
32	Geometric Approach to Response Theory in Non-Hamiltonian Systems. Journal of Mathematical Chemistry, 2002, 32, 339-360.	0.7	13
33	Eigenstate assignments and the quantum-classical correspondence for highly-excited vibrational states of the Baggot H2O Hamiltonian. Journal of Chemical Physics, 1997, 107, 156-179.	1.2	57
34	Periodic orbit analysis of molecular vibrational spectra: Spectral patterns and dynamical bifurcations in Fermi resonant systems. Journal of Chemical Physics, 1996, 104, 26-35.	1.2	30
35	Periodic orbit analysis of molecular vibrational spectra: 1:1 resonant coupled modes. Journal of Chemical Physics, 1995, 103, 1375-1383.	1.2	16
36	Vibrationally induced rotational axis switching: A novel mechanism for vibrational mode coupling. Journal of Chemical Physics, 1992, 97, 5956-5963.	1.2	27

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37	Vibrational deactivation in Kr/O2+collisions: Role of complex formation and potential anisotropy. Journal of Chemical Physics, 1992, 97, 6322-6334.	1.2	18
38	Transport and turnstiles in multidimensional Hamiltonian mappings for unimolecular fragmentation: Application to van der Waals predissociation. Journal of Chemical Physics, 1991, 94, 2648-2668.	1.2	86
39	Avoided crossings and resummation of nearly resonant molecular vibrations: Reconstruction of an effective secular equation. Journal of Chemical Physics, 1989, 90, 6378-6390.	1.2	25
40	Classical, quantum mechanical, and semiclassical representations of resonant dynamics: A unified treatment. Journal of Chemical Physics, 1987, 87, 284-302.	1.2	41
41	Classical and semiclassical mechanics of strongly resonant systems: A Fourier transform approach. Journal of Chemical Physics, 1987, 86, 279-307.	1.2	118
42	Semiclassical quantization using classical perturbation theory: Algebraic quantization of multidimensional systems. Journal of Chemical Physics, 1987, 86, 6270-6282.	1.2	134
43	PERTURB: A special-purpose algebraic manipulation program for classical perturbation theory. Journal of Computational Chemistry, 1987, 8, 397-411.	1.5	9
44	Semiclassical quantization of a classical analog for the Jahnâ€“TellerEÃ—esystem. Journal of Chemical Physics, 1986, 85, 2089-2098.	1.2	26
45	Intramolecular dynamics and multiresonant absorption spectroscopy. II. Power broadening and superposition states in double resonant twoâ€photon excitation. Journal of Chemical Physics, 1985, 83, 5369-5379.	1.2	15
46	EBK quantization of nonseparable systems: A Fourier transform method. Journal of Chemical Physics, 1985, 83, 2990-3001.	1.2	126