Lionel M Raff

List of Publications by Year
in descending order

58	1,011	393982	476904
papers	citations	19 h-index	29 g-index

59	59	59	369
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Projection methods for obtaining intramolecular energy transfer rates from classical trajectory results: Application to 1,2â€difluoroethane. Journal of Chemical Physics, 1988, 89, 5680-5691.	1.2	61
2	Statistical and nonstatistical effects in bond fission reactions of SiH2 and Si2H6. Journal of Chemical Physics, 1991, 94, 4219-4229.	1.2	50
3	Monte Carlo variational transitionâ€state theory study of recombination and desorption of hydrogen on Si(111). Journal of Chemical Physics, 1986, 85, 3081-3089.	1.2	45
4	Theoretical studies of the reaction dynamics of the matrixâ€isolated F2+cisâ€d2 â€ethylene system. Journal of Chemical Physics, 1991, 95, 8901-8918.	1.2	44
5	Diffusion of H atoms on a Si(111) surface with partial hydrogen coverage: Monte Carlo variational phaseâ€space theory with tunneling correction. Journal of Chemical Physics, 1988, 88, 7221-7231.	1.2	42
6	Comparisons of statistical and nonstatistical behavior for bond fission reactions in 1,2â€difluoroethane, disilane, and the 2â€chloroethyl radical. Journal of Chemical Physics, 1991, 95, 8089-8107.	1.2	41
7	Theoretical studies of hydrogenâ€abstraction reactions from diamond and diamondâ€like surfaces. Journal of Chemical Physics, 1993, 99, 4748-4758.	1.2	41
8	Monte Carlo simulations of void-nucleated melting of silicon via modification in the Tersoff potential parameters. Physical Review B, 2005, 72, .	1.1	40
9	Unimolecular dissociation dynamics of disilane. Journal of Chemical Physics, 1990, 92, 1069-1082.	1.2	38
10	Intramolecular energy transfer and modeâ€specific effects in unimolecular reactions of 1,2â€difluoroethane. Journal of Chemical Physics, 1989, 90, 6313-6319.	1.2	36
11	Energy transfer and reaction dynamics of matrixâ€isolated 1,2â€difluoroethaneâ€d4. Journal of Chemical Physics, 1990, 93, 3160-3176.	1.2	36
12	Intramolecular energy transfer and modeâ€specific effects in unimolecular reactions of disilane. Journal of Chemical Physics, 1991, 95, 106-120.	1.2	36
13	Molecular dynamics studies of the thermal decomposition of 2,3â€diazabicyclo(2.2.1)heptâ€2â€ene. Journal of Chemical Physics, 1995, 102, 7910-7924.	1.2	27
14	The dynamics of dissociative chemisorption of H2 on a Si(111) surface. Journal of Chemical Physics, 1987, 86, 1608-1615.	1.2	25
15	Computational studies of SiH2+SiH2 recombination reaction dynamics on a global potential surface fitted to ab initio and experimental data. Journal of Chemical Physics, 1988, 88, 5948-5962.	1.2	23
16	Statistical and Nonstatistical Dynamics in the Unimolecular Decomposition of Vinyl Bromide. Journal of Physical Chemistry A, 1997, 101, 1007-1017.	1.1	23
17	Theoretical studies of the effects of matrix composition, lattice temperature, and isotopic substitution on isomerization reactions of matrixâ€isolated HONO/Ar. Journal of Chemical Physics, 1995, 102, 7000-7005.	1.2	22
18	Theoretical studies of termolecular thermal recombination of silicon atoms. Journal of Chemical Physics, 1986, 84, 4426-4428.	1.2	21

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19	Trajectory Investigations of the Dissociation Dynamics of Vinyl Bromide on an ab Initio Potential-Energy Surface. Journal of Physical Chemistry A, 2001, 105, 2156-2172.	1.1	21
20	Monte Carlo random walk study of recombination and desorption of hydrogen on Si(111). Journal of Chemical Physics, 1985, 83, 1382-1391.	1.2	18
21	Theoretical investigation of nonstatistical dynamics, energy transfer, and intramolecular vibrational relaxation in isomerization reactions of matrixâ€isolated HONO/Xe. Journal of Chemical Physics, 1994, 101, 9937-9945.	1.2	18
22	Variational phaseâ€space theory studies of siliconâ€atom diffusion on reconstructed Si(111)â€(7Ã—7) surfaces. Journal of Chemical Physics, 1989, 91, 6463-6471.	1.2	17
23	Effects of lattice morphology upon reaction dynamics in matrixâ€isolated systems. Journal of Chemical Physics, 1992, 97, 7459-7470.	1.2	17
24	Spontaneity and Equilibrium: Why â€œÎ”G < 0 Denotes a Spontaneous Processâ€•and â€œÎ”G = 0 Means the System Is at Equilibriumâ€•Are Incorrect. Journal of Chemical Education, 2014, 91, 386-395.	1.1	17
25	Trajectory studies of unimolecular reactions of Si2H4 and SiH2 on a global potential surface fitted to ab initio and experimental data. Journal of Chemical Physics, 1988, 89, 741-750.	1.2	16
26	Hydrogenâ€atom migration on a diamond (111) surface. Journal of Chemical Physics, 1994, 100, 1765-1766.	1.2	16
27	Statistical effects in the skeletal inversion of bicyclo(2.1.0) pentane. Journal of Chemical Physics, 1994, 101, 3729-3741.	1.2	16
28	Diffusion of hydrogen atoms on a Si(111)â€(7Ã—7) reconstructed surface: Monte Carlo variational phaseâ€space theory. Journal of Chemical Physics, 1994, 101, 1638-1647.	1.2	15
29	Theoretical Investigations of Intramolecular Energy Transfer Rates and Pathways for Vinyl Bromide on an ab Initio Potential-Energy Surface. Journal of Physical Chemistry A, 2001, 105, 2147-2155.	1.1	15
30	Dynamics of unimolecular dissociation of silylene. Journal of Chemical Physics, 1986, 84, 4341-4346.	1.2	13
31	Trajectory study of the formation and decay of silicon trimer complexes in monomerâ€“dimer collisions. Journal of Chemical Physics, 1988, 88, 156-162.	1.2	13
32	Effect of lattice potential upon the surface diffusion of Si on Si(100). Journal of Chemical Physics, 1985, 83, 6009-6011.	1.2	11
33	Wave packet studies of gasâ€“surface inelastic scattering and desorption rates. Journal of Chemical Physics, 1988, 88, 1264-1271.	1.2	11
34	Power spectra as a diagnostic tool in probing statistical/nonstatistical behavior in unimolecular reactions. Journal of Chemical Physics, 1992, 97, 7354-7361.	1.2	11
35	Solvent Dimer Model for Solvated Electrons. Advances in Chemistry Series, 1965, , 173-179.	0.6	10
36	Classical trajectory study of the unimolecular dissociation of ammonia. Journal of Chemical Physics, 1986, 85, 4392-4399.	1.2	9

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37	Classical Variational Transition State Theory Study of Hydrogen Atom Diffusion Dynamics in Imperfect Xenon Matrices. Journal of Physical Chemistry A, 1997, 101, 235-242.	1.1	9
38	Computational studies of heterogeneous reactions of SiH2 on reconstructed Si(111)â€“(7Ã—7) and Si(111)â€“(1Ã—1) surfaces. Journal of Chemical Physics, 1989, 91, 5021-5029.	1.2	8
39	Silicon dimer formation by threeâ€body recombination. Journal of Chemical Physics, 1990, 92, 5311-5318.	1.2	8
40	Trajectory study of Si4 formation and decay and of exchange and abstraction reactions in Si+Si3 collisions. Journal of Chemical Physics, 1990, 93, 6607-6619.	1.2	8
41	Statistical effects in the thermal deazetization reaction of 2,3â€diazabicyclo(2.2.1)heptâ€2â€ene. Journal of Chemical Physics, 1995, 103, 5387-5393.	1.2	8
42	Intramolecular Energy Transfer Rates and Pathways for Vinyl Bromide. The Journal of Physical Chemistry, 1996, 100, 8085-8092.	2.9	8
43	Spontaneity and Equilibrium II: Multireaction Systems. Journal of Chemical Education, 2014, 91, 839-847.	1.1	8
44	A perturbationâ€“trajectory method for the study of gasâ€“surface collision dynamics. Journal of Chemical Physics, 1989, 90, 3363-3372.	1.2	7
45	Comparison of siliconâ€atom diffusion on the dimerâ€“adatomâ€stacking fault and Binnig et al. models of the reconstructed Si(111)â€(7Ã—7) surface. Journal of Chemical Physics, 1991, 94, 6243-6249.	1.2	7
46	Chemical and biochemical thermodynamics: Is it time for a reunification?. Biophysical Chemistry, 2017, 221, 49-57.	1.5	6
47	Theoretical studies of vibrationally assisted reactions of the O3â€‰â‹…â€‰NO van der Waals complex. Journal of Chemical Physics, 1986, 84, 3803-3813.	1.2	5
48	GEOMETRICAL OPTIMIZATIONS, NMR ANALYSES, AND NOVEL CRYSTAL STRUCTURES OF 3-OXA-7-BENZYL-7-AZABICYCLO[3.3.1]-NONAN-9-ONE AND 3-THIA-7-BENZYL-7-AZABICYCLO[3.3.1]-NONAN-9-ONE; STRUCTURAL ANALYSIS OF THE CORRESPONDING 3,7-DIHETERABICYCLO[3.3.l]NONANE HYDROPERCHLORATES. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 148, 97-116.	0.8	4
49	Spontaneity and Equilibrium III: A History of Misinformation. Journal of Chemical Education, 2014, 91, 2128-2136.	1.1	3
50	Intramolecular energy transfer rates for vinyl bromide and deuterium-substituted vinyl bromides from power spectrum line splittings. Journal of Chemical Physics, 1997, 106, 1382-1390.	1.2	2
51	Are the Concepts of Dynamic Equilibrium and the Thermodynamic Criteria for Spontaneity, Nonspontaneity, and Equilibrium Compatible?. Journal of Chemical Education, 2015, 92, 655-659.	1.1	2
52	On the Reunification of Chemical and Biochemical Thermodynamics: A Simple Example for Classroom Use. Journal of Chemical Education, 2019, 96, 274-284.	1.1	2
53	Solution Mixing Calculations for Saturated ACâ€“BC Solutions: A General Analytical Analysis. Journal of Chemical Education, 2021, 98, 1667-1672.	1.1	1
54	Reply to the â€˜â€˜Comment on silane pyrolysis and the insertion of silylene into molecular hydrogenâ€™â€™. Journal of Chemical Physics, 1987, 86, 3058-3058.	1.2	0

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55	Comment on â€˜â€˜A perturbationâ€“trajectory method for the study of gasâ€“surface collision dynamicsâ€™â€™. Journal of Chemical Physics, 1990, 92, 817-818.	1.2	0
56	Theoretical Investigations of Chemical and Physical Processes under Matrix Isolation Conditions. , 1998, , 266-354.		0
57	A network pruning algorithm for combined function and derivative approximation. , 2009, , .		0
58	The formulation of chemical potentials and free energy changes in biochemical reactions. Physical Chemistry Chemical Physics, 2021, 23, 14783-14795.	1.3	0