Richard L Jaffe

List of Publications by Year
in descending order

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63 papers	4,169 citations	159358 30 h-index	182168 51 g-index
65 all docs	65 docs citations	65 times ranked	2427 citing authors

#	Article	IF	Citations
1	Review of chemical-kinetic problems of future NASA missions. II - Mars entries. Journal of Thermophysics and Heat Transfer, 1994, 8, 9-23.	0.9	660
2	Chemical-Kinetic Parameters of Hyperbolic Earth Entry. Journal of Thermophysics and Heat Transfer, 2001, 15, 76-90.	0.9	423
3	A quantum chemistry study of benzene dimer. Journal of Chemical Physics, 1996, 105, 2780-2788.	1.2	273
4	Molecular Dynamics Simulation of Contact Angles of Water Droplets in Carbon Nanotubes. Nano Letters, 2001, 1, 697-702.	4.5	230
5	Low-Dielectric, Nanoporous Organosilicate Films Prepared via Inorganic/Organic Polymer Hybrid Templates. Chemistry of Materials, 1999, 11, 3080-3085.	3.2	214
6	Rovibrational internal energy transfer and dissociation of $mathbf { m N_2(^1Sigma _g^+)-m N(^4S_u)}$N2(1Î£g+)â^'N(4Su) system in hypersonic flows. Journal of Chemical Physics, 2013, 138, 044312.	1.2	208
7	Conformations and Structures of Poly(oxyethylene) Melts from Molecular Dynamics Simulations and Small-Angle Neutron Scattering Experiments. Macromolecules, 1996, 29, 3462-3469.	2.2	165
8	Force field for simulations of 1,2-dimethoxyethane and poly(oxyethylene) based upon ab initio electronic structure calculations on model molecules. The Journal of Physical Chemistry, 1993, 97, 12752-12759.	2.9	149
9	Conformation of 1,2-dimethoxyethane from ab initio electronic structure calculations. The Journal of Physical Chemistry, 1993, 97, 12745-12751.	2.9	135
10	Classical Trajectory Analysis of the Reaction F+H2â†'HF+H. Journal of Chemical Physics, 1971, 54, 2224-2236.	1.2	123
11	Quantum Chemistry Study of Conformational Energies and Rotational Energy Barriers inn-Alkanes. The Journal of Physical Chemistry, 1996, 100, 18718-18724.	2.9	118
12	Coarse-grain model for internal energy excitation and dissociation of molecular nitrogen. Chemical Physics, 2012, 398, 90-95.	0.9	87
13	Conformational Characteristics of Poly(tetrafluoroethylene) Chains Based upon ab Initio Electronic Structure Calculations on Model Molecules. Macromolecules, 1994, 27, 3166-3173.	2.2	77
14	Conformations and order in atactic poly(vinyl chloride) melts from molecular dynamics simulations. Macromolecules, 1993, 26, 298-304.	2.2	76
15	Ab initio quantum chemistry and molecular dynamics simulations studies of LiPF6/poly(ethylene oxide) interactions. Journal of Computational Chemistry, 2001, 22, 641-654.	1.5	76
16	Waterâ€"Carbon Interactions 2: Calibration of Potentials using Contact Angle Data for Different Interaction Models. Molecular Simulation, 2004, 30, 205-216.	0.9	72
17	Comparative Study of Force Fields for Benzene. The Journal of Physical Chemistry, 1996, 100, 9624-9630.	2.9	70
18	Theoretical studies of the potential surface for the F+H2â†'HF+H reaction. Journal of Chemical Physics, 1988, 88, 1743-1751.	1.2	69

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19	Total integral reactive cross sections for F + H2 â†' HF + H: comparison of converged quantum, quasiclassical trajectory and experimental results. Chemical Physics Letters, 1991, 176, 546-550.	1.2	68
20	Conformations of 1,2-Dimethoxyethane in the Gas and Liquid Phases from Molecular Dynamics Simulations. Journal of the American Chemical Society, 1995, 117, 530-531.	6.6	66
21	A third-order rotational isomeric state model for poly(oxyethylene) based upon ab initio electronic structure analyses of model molecules. Macromolecules, 1993, 26, 5213-5218.	2.2	61
22	Quantum Chemistry Study of the Interactions of Li+, Cl-, and I-Ions with Model Ethers. Journal of Physical Chemistry A, 1997, 101, 1705-1715.	1.1	60
23	MCSCF potential energy surface for photodissociation of formaldehyde. Journal of Chemical Physics, 1976, 64, 4881-4886.	1.2	48
24	Structure and properties of polymethylene melt surfaces from molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 2831-2840.	1.2	46
25	Dynamics of poly(oxyethylene) melts: Comparison of 13C nuclear magnetic resonance spin-lattice relaxation and dielectric relaxation as determined from simulations and experiments. Journal of Chemical Physics, 1997, 106, 3798-3805.	1.2	44
26	Ab initio and semiempirical study of multiple surfaces and their analytic continuation for collinear F(2P3/2, 2P1/2)+H2â†'FH+H. Journal of Chemical Physics, 1975, 63, 3417-3424.	1.2	42
27	Conformational Characteristics of Dimethoxymethane Based upon ab Initio Electronic Structure Calculations. The Journal of Physical Chemistry, 1994, 98, 9072-9077.	2.9	41
28	Long-Time Molecular Motions and Local Chain Dynamics in n-C44H90 Melts by Molecular Dynamics Simulations. Macromolecules, 1995, 28, 5897-5905.	2.2	40
29	AB initio calculation of the two-photon absorption cross section of the X 1 Î£g+ â†' (E,F) 1 Î£g+ IN H2. Chemical Physics Letters, 1983, 101, 463-471.	1.2	33
30	Comparison of Potential Energy Surface and Computed Rate Coefficients for N2 Dissociation. Journal of Thermophysics and Heat Transfer, 2018, 32, 869-881.	0.9	33
31	Conformational Characteristics of Polymethylene Chains in Melts and in Various Phantom Chains from Explicit Atom Molecular Dynamics Simulations. Macromolecules, 1997, 30, 7245-7252.	2.2	30
32	Polymer force fields from ab initio studies of small model molecules: can we achieve chemical accuracy?. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1997, 53, 1273-1283.	2.0	29
33	First Principles Calculation of Heavy Particle Rate Coefficients. , 2015, , 103-158.		25
34	Conformations of 2,4-Diphenylpentane:Â A Quantum Chemistry and Gas-Phase Molecular Dynamics Simulation Study. Journal of Physical Chemistry A, 1998, 102, 4694-4702.	1.1	20
35	Dissociation and internal excitation of molecular nitrogen due to N2-N collisions using direct molecular simulation. , 2017, , .		20
36	Conformations of 2,4-Dichloropentane and 2,4,6-Trichloroheptane and a Force Field for Poly(vinyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 1995, 99, 164-172.	2.9	19

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37	Thermodynamic properties of carbonâ€“phenolic gas mixtures. Aerospace Science and Technology, 2017, 66, 177-192.	2.5	19
38	Conformational Characteristics of Poly(oxymethylene) Based upon ab Initio Electronic Structure Calculations. The Journal of Physical Chemistry, 1994, 98, 9078-9082.	2.9	14
39	Calculations of potential energy surfaces in the complex plane. IV. Ab initio surfaces for H3+. Journal of Chemical Physics, 1974, 61, 4717-4725.	1.2	13
40	Calculations of potential energy surfaces in the complex plane. Molecular Physics, 1974, 28, 1489-1503.	0.8	13
41	Effective cross sections and rate constants for predissociation of ClO in the earth's atmosphere. Journal of Quantitative Spectroscopy and Radiative Transfer, 1977, 18, 227-235.	1.1	13
42	Conformational Characteristics of 1,3-Dimethoxypropane and Poly(oxytrimethylene) Based upon ab Initio Electronic Structure Calculations. The Journal of Physical Chemistry, 1996, 100, 13439-13446.	2.9	13
43	Classical Trajectory Studies of Gas Phase Reaction Dynamics and Kinetics Using Ab initio Potential Energy Surfaces. , 1989, , 367-382.		13
44	Comparison of quantum mechanical and empirical potential energy surfaces and computed rate coefficients for N2 dissociation. , 2016, , .		12
45	Ab InitioCalculation of the Third-Order Susceptibility ofH2. Physical Review Letters, 1981, 47, 30-34.	2.9	11
46	Conformations of 1,2-dimethoxypropane and 5-methoxy-1,3-dioxane: are ab initio quantum chemistry predictions accurate?. Chemical Physics Letters, 1998, 289, 480-486.	1.2	10
47	Surface and Thin Film Characteristics of Poly(tetrafluoroethylene) Melts from Molecular Dynamics Simulations. Macromolecules, 2007, 40, 7407-7412.	2.2	10
48	Calculated rate constants for the reaction ClO + O â† Cl + O2 between 220 and 1000 k. Chemical Physics, 1979, 40, 185-206.	0.9	9
49	State-resolved transport collision integrals for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">O</mml:mi><mml:mo>+</mml:mo><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> system. Physical Review Fluids, 2020, 5, .	1.0	8
50	Quantum Chemistry Study of Li+âˆ'1,2-Dimethoxypropane Complexes. Journal of Physical Chemistry A, 1997, 101, 3152-3157.	1.1	7
51	Energy transfer study of N2-N2 interactions by using rovibrational state-to-state model. , 2013, , .		7
52	On the development of a new nonequilibrium chemistry model for Mars entry. , 2017, , .		7
53	Ab initio based rovibrational grouping model for N₂(¹Î£⁺) Tj ETQq1 1 0.784314 rgBT /Overloc dissociation. , 2017, , .		5
54	Comment on the relation between the nonadiabatic coupling and the complex intersection of potential energy curves. Chemical Physics, 1977, 23, 249-255.	0.9	4

#	Article	IF	Citations
55	Dissociation and Energy transfer study of N2-N and N2-N2 interactions by using rovibrational and coarse-grained state-to-state models. , 2015, , .		4
56	The Effect of the Spin-forbidden CO (1Î£+) + O (3P) â† CO2 (1Î£g+) Recombination Reaction on Afterbody Heating of Mars Entry Vehicles. , 2017, , .		4
57	Coarse-grain cross sections for rovibrational excitation and dissociation of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si58.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mo linebreak="badbreak">-</mml:mo><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> system. Chemical Physics, 2020, 533, 110758.	2.0	3
58	Calculations of potential energy surfaces in the complex plane. Theoretica Chimica Acta, 1975, 40, 189-197.	0.9	2
59	Carbon Clusters: Thermochemistry and Electronic Structure at High Temperatures. Journal of Physical Chemistry A, 2021, 125, 7038-7051.	1.1	2
60	Calculation of Thermochemical Properties of Carbon-cluster Ablation Species. , 2018, , .		1
61	Importance of Exchange Processes in Earth and Mars Atmospheric Kinetics: Application to HCN System. , 2022, , .		1
62	Semiclassical Study of the Quenching of Excitedâ€State Fluorine Atom by Hydrogen Molecule: Comparison between Reactive and Nonreactive Processes. Israel Journal of Chemistry, 1980, 19, 337-339.	1.0	0
63	Hybrid reduced order model for N2-N interactions for application to dissociation and energy transfer processes. AIP Conference Proceedings, 2019, , .	0.3	0