Karl F Freed

List of Publications by Year
in descending order

616	21,348	10389 72	30922 102
papers	citations	h-index	g-index

626	626	626	7760
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Multiphonon Processes in the Nonradiative Decay of Large Molecules. Journal of Chemical Physics, 1970, 52, 6272-6291.	3.0	526
2	Characterization of branching architecture through "universal" ratios of polymer solution properties. Macromolecules, 1990, 23, 4168-4180.	4.8	304
3	Statistical coil model of the unfolded state: Resolving the reconciliation problem. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13099-13104.	7.1	290
4	Effect of monomer structure and compressibility on the properties of multicomponent polymer blends and solutions: 1. Lattice cluster theory of compressible systems. Macromolecules, 1991, 24, 5076-5095.	4.8	246
5	Functional Integrals and Polymer Statistics. Advances in Chemical Physics, 2007, , 1-128.	0.3	228
6	Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water. Science, 2017, 358, 238-241.	12.6	194
7	Analysis and Evaluation of Ionization Potentials, Electron Affinities, and Excitation Energies by the Equations of Motion-Green's Function Method. Advances in Chemical Physics, 2007, , 1-69.	0.3	185
8	Dependence of Radiationless Decay Rates in Polyatomic Molecules upon the Initially Selected Vibronic State: General Theory and Application. Journal of Chemical Physics, 1972, 56, 2309-2328.	3.0	179
9	Polymer viscosity in concentrated solutions. Journal of Chemical Physics, 1974, 61, 3626-3633.	3.0	175
10	Theory of the Hyperfine Structure of Molecules: Application to 3Î States of Diatomic Molecules Intermediate between Hund's Cases (a) and (b). Journal of Chemical Physics, 1966, 45, 4214-4241.	3.0	170
11	Helix, Sheet, and Polyproline II Frequencies and Strong Nearest Neighbor Effects in a Restricted Coil Library. Biochemistry, 2005, 44, 9691-9702.	2.5	165
12	The Glass Transition Temperature of Polymer Melts. Journal of Physical Chemistry B, 2005, 109, 21285-21292.	2.6	157
13	Intramolecular vibrational energy redistribution and the time evolution of molecular fluorescence. Journal of Chemical Physics, 1980, 73, 4765-4778.	3.0	156
14	Systematic corrections to Floryâ€“Huggins theory: Polymerâ€“solventâ€“void systems and binary blendâ€“void systems. Journal of Chemical Physics, 1988, 88, 2741-2756.	3.0	149
15	Role of molecular structure on the thermodynamic properties of melts, blends, and concentrated polymer solutions: comparison of Monte Carlo simulations with the cluster theory for the lattice model. Macromolecules, 1990, 23, 4803-4819.	4.8	147
16	Intramolecular perturbations and the quenching of luminescence in small molecules. Chemical Physics Letters, 1973, 18, 470-475.	2.6	141
17	Theory of the dynamical viscosity of polymer solutions. Journal of Chemical Physics, 1974, 61, 1189-1202.	3.0	138
18	Theory of diatomic molecule photodissociation: Electronic angular momentum influence on fragment and fluorescence cross sections. Journal of Chemical Physics, 1983, 79, 6060-6085.	3.0	135

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19	Hydrodynamic theory for vibrational relaxation in liquids. Physical Review A, 1977, 15, 361-371.	2.5	132
20	Effect of monomer structure and compressibility on the properties of multicomponent polymer blends and solutions. 2. Application to binary blends. Macromolecules, 1991, 24, 5096-5111.	4.8	132
21	Internal Rotation and the Breakdown of the Adiabatic Approximation: Manyâ€Phonon Radiationless Transitions. Journal of Chemical Physics, 1970, 52, 2460-2473.	3.0	126
22	Renormalization and the two-parameter theory. Macromolecules, 1984, 17, 2344-2354.	4.8	124
23	Effect of monomer structure and compressibility on the properties of multicomponent polymer blends and solutions. 3. Application to deuterated polystyrene [PS(D)]poly(vinyl methyl ether) (PVME) blends. Macromolecules, 1991, 24, 5112-5123.	4.8	122
24	Fragility of Glass-Forming Polymer Liquids. Journal of Physical Chemistry B, 2005, 109, 21350-21356.	2.6	121
25	Dissociation processes of polyatomic molecules. Journal of Chemical Physics, 1975, 63, 3382-3397.	3.0	120
26	Radiationless transitions in molecules. Accounts of Chemical Research, 1978, 11, 74-80.	15.6	118
27	Investigations into Sequence and Conformational Dependence of Backbone Entropy, Inter-basin Dynamics and the Flory Isolated-pair Hypothesis for Peptides. Journal of Molecular Biology, 2003, 331, 693-711.	4.2	118
28	Lattice model of living polymerization. I. Basic thermodynamic properties. Journal of Chemical Physics, 1999, 111, 7116-7130.	3.0	114
29	Phase equilibria of lattice polymer and solvent: tests of theories against simulations. Macromolecules, 1990, 23, 1181-1191.	4.8	112
30	Positional time correlation function for oneâ€dimensional systems with barrier crossing: Memory function corrections to the optimized Rouseâ€“Zimm approximation. Journal of Chemical Physics, 1993, 98, 564-573.	3.0	112
31	Relation of effective interaction parameters for binary blends and diblock copolymers: lattice cluster theory predictions and comparisons with experiment. Macromolecules, 1993, 26, 213-220.	4.8	108
32	Long Time Dynamics of Met-Enkephalin: Comparison of Explicit and Implicit Solvent Models. Biophysical Journal, 2002, 82, 1791-1808.	0.5	108
33	Analysis of ab initio effective valence shell Hamiltonian calculations using third order quasidegenerate manyâ€body perturbation theory. Journal of Chemical Physics, 1981, 75, 4507-4524.	3.0	102
34	Excluded volume in star polymers: chain conformation space renormalization group. Macromolecules, 1983, 16, 1228-1241.	4.8	102
35	Loss of conformational entropy in protein folding calculated using realistic ensembles and its implications for NMR-based calculations. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15396-15401.	7.1	101
36	Radiative Decay of Polyatomic Molecules. Journal of Chemical Physics, 1969, 50, 2916-2927.	3.0	100

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37	A lattice field theory for polymer systems with nearestâ€neighbor interaction energies. Journal of Chemical Physics, 1987, 87, 5534-5540.	3.0	97
38	All-atom fast protein folding simulations: The villin headpiece. Proteins: Structure, Function and Bioinformatics, 2002, 49, 439-445.	2.6	97
39	Is there a bridge between ab initio and semiempirical theories of valence?. Accounts of Chemical Research, 1983, 16, 137-144.	15.6	96
40	Lattice theories of polymeric fluids. The Journal of Physical Chemistry, 1989, 93, 2194-2203.	2.9	96
41	Theoretical foundations of purely semiempirical quantum chemistry. Journal of Chemical Physics, 1974, 60, 1765-1788.	3.0	95
42	Halfâ€collision description of final state distributions of the photodissociation of polyatomic molecules. Journal of Chemical Physics, 1981, 74, 4380-4394.	3.0	95
43	Ab initio study of the transâ€butadiene Ï€â€valence states using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 1992, 96, 1304-1316.	3.0	95
44	The improved virtual orbital-complete active space configuration interaction method, a â€œpackageableâ€• efficientab initiomany-body method for describing electronically excited states. Journal of Chemical Physics, 2001, 114, 2592-2600.	3.0	95
45	Ab initio evaluation of correlation contributions to the true Ï€â€electron Hamiltonian: Ethylene. Journal of Chemical Physics, 1974, 61, 1500-1509.	3.0	93
46	Theory of collision induced intersystem crossing. Journal of Chemical Physics, 1976, 64, 1604-1611.	3.0	93
47	Lattice models of polymer solutions: Monomers occupying several lattice sites. Journal of Chemical Physics, 1987, 87, 7272-7284.	3.0	93
48	Applications of multireference perturbation theory to potential energy surfaces by optimal partitioning ofH: Intruder states avoidance and convergence enhancement. Journal of Chemical Physics, 1995, 103, 4990-5010.	3.0	93
49	Application of the entropy theory of glass formation to poly(Î±-olefins). Journal of Chemical Physics, 2009, 131, 114905.	3.0	93
50	Irreversible Electronic Relaxation in Polyatomic Molecules. Journal of Chemical Physics, 1970, 52, 1345-1354.	3.0	88
51	Theta point (â€˜â€˜tricriticalâ€™â€™) region behavior for a polymer chain: Transition to collapse. Journal of Chemical Physics, 1984, 80, 900-924.	3.0	87
52	Lattice model of equilibrium polymerization. IV. Influence of activation, chemical initiation, chain scission and fusion, and chain stiffness on polymerization and phase separation. Journal of Chemical Physics, 2003, 119, 12645-12666.	3.0	87
53	A one-dimensional microscopic quantum mechanical theory of light enhanced desorption. Surface Science, 1981, 109, 191-206.	1.9	85
54	Influence of Short Chain Branching on the Miscibility of Binary Polymer Blends:â€‰ Application to Polyolefin Mixtures. Macromolecules, 1996, 29, 625-636.	4.8	85

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55	Entropy theory of polymer glass formation revisited. I. General formulation. Journal of Chemical Physics, 2006, 124, 064901.	3.0	85
56	Cluster Theory of the Electronic Structure of Disordered Systems. Physical Review B, 1971, 3, 3400-3417.	3.2	83
57	Wiener Integrals and Models of Stiff Polymer Chains. Journal of Chemical Physics, 1971, 54, 1453-1463.	3.0	80
58	Interfacial studies of incompressible binary blends. Journal of Chemical Physics, 1991, 94, 6307-6322.	3.0	80
59	Communication: Cosolvency and cononsolvency explained in terms of a Flory-Huggins type theory. Journal of Chemical Physics, 2015, 143, 131101.	3.0	79
60	Rotational distributions from photodissociations. I. Linear triatomic molecules. Journal of Chemical Physics, 1979, 70, 3604-3619.	3.0	78
61	Anomalous isotope dependence of hydrogen diffusion rates on tungsten (110) surfaces: Implications for latticeâ€“hydrogen interactions. Journal of Chemical Physics, 1987, 86, 2356-2361.	3.0	78
62	Penetration function and second virial coefficient for linear and regular star polymers. Macromolecules, 1984, 17, 1854-1870.	4.8	77
63	Free energy functional expansion for inhomogeneous polymer blends. Journal of Chemical Physics, 1991, 94, 1572-1583.	3.0	77
64	Ab initio effective valence shell Hamiltonian for the neutral and ionic valence states of N, O, F, Si, P, and S. Journal of Chemical Physics, 1980, 72, 4158-4173.	3.0	76
65	Plasticization and antiplasticization of polymer melts diluted by low molar mass species. Journal of Chemical Physics, 2010, 132, 084504.	3.0	76
66	Does equilibrium polymerization describe the dynamic heterogeneity of glass-forming liquids?. Journal of Chemical Physics, 2006, 125, 144907.	3.0	75
67	Rotational distributions from photodissociation. II. Results for ICN+hÎ½â†'l+CN(Xâ€‰2Î£+). Journal of Chemical Physics, 1979, 70, 3620-3629.	3.0	74
68	Conformation space renormalization of polymers. II. Single chain dynamics based on chain diffusion equation model. Journal of Chemical Physics, 1981, 75, 1009-1015.	3.0	74
69	Application of dimensional regularization to single chain polymer static properties: Conformational space renormalization of polymers. III. Journal of Chemical Physics, 1981, 74, 6458-6466.	3.0	74
70	Lattice model of living polymerization. III. Evidence for particle clustering from phase separation properties and â€œroundingâ€•of the dynamical clustering transition. Journal of Chemical Physics, 2000, 113, 434-446.	3.0	74
71	A lattice model for selfâ€avoiding polymers with controlled length distributions. II. Corrections to Floryâ€“Huggins mean field. Journal of Chemical Physics, 1986, 84, 7036-7047.	3.0	73
72	Boltzmann statistics and radiationless decay in large molecules: Optical selection studies. Chemical Physics Letters, 1970, 6, 345-351.	2.6	72

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73	On the Stokes problem for a suspension of spheres at finite concentrations. Journal of Chemical Physics, 1978, 68, 2088-2096.	3.0	72
74	Pressure Dependence of Polymer Fluids: Application of the Lattice Cluster Theory. Macromolecules, 1995, 28, 6625-6641.	4.8	72
75	A density functional theory of polymer phase transitions and interfaces. Journal of Chemical Physics, 1990, 92, 1413-1426.	3.0	71
76	Many-Body Approach to Electron Correlation in Atoms and Molecules. Physical Review, 1968, 173, 1-24.	2.7	67
77	Effect of residual interactions on polymer properties near the theta point. Journal of Chemical Physics, 1985, 83, 5293-5310.	3.0	67
78	Influence of Monomer Molecular Structure on the Miscibility of Polymer Blends. , 0, , 63-126.		67
79	Benchmarking all-atom simulations using hydrogen exchange. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15975-15980.	7.1	67
80	Nonradiative decay processes in benzene. Chemical Physics, 1974, 6, 331-352.	1.9	66
81	A oneâ€dimensional model for phononâ€induced desorption. Journal of Chemical Physics, 1983, 79, 2436-2453.	3.0	66
82	Modeling the Hydration Layer around Proteins: Applications to Small- and Wide-Angle X-Ray Scattering. Biophysical Journal, 2011, 101, 2061-2069.	0.5	66
83	Rotational mechanism for vibrational relaxation in rigid media. Chemical Physics Letters, 1977, 48, 262-266.	2.6	65
84	Lattice model of equilibrium polymerization. VII. Understanding the role of â€œcooperativityâ€•in self-assembly. Journal of Chemical Physics, 2008, 128, 224901.	3.0	65
85	Influence of Cohesive Energy on the Thermodynamic Properties of a Model Glass-Forming Polymer Melt. Macromolecules, 2016, 49, 8341-8354.	4.8	65
86	Path Integrals and Semiclassical Tunneling, Wavefunctions, and Energies. Journal of Chemical Physics, 1972, 56, 692-697.	3.0	64
87	Theory of Concentration Dependence of Polymer Relaxation Times in Dilute Solutions. Macromolecules, 1978, 11, 843-852.	4.8	64
88	Rotational and angular distributions from photodissociations. III. Effects of dynamic axis switching in linear triatomic molecules. Journal of Chemical Physics, 1981, 74, 4395-4417.	3.0	64
89	A Wiener integral model for stiff polymer chains. Journal of Chemical Physics, 1985, 83, 2491-2496.	3.0	64
90	Flory-Huggins Model of Equilibrium Polymerization and Phase Separation in the Stockmayer Fluid. Physical Review Letters, 2004, 92, 045502.	7.8	64

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91	Nonclassical terms in the true effective valence shell Hamiltonian: A second quantized formalism. Journal of Chemical Physics, 1976, 65, 1071-1088.	3.0	63
92	Convergence studies of the effective valence shell Hamiltonian for correlation energies of the fluorine atom and its ions using third order quasidegenerate manyâ€body perturbation theory. Journal of Chemical Physics, 1981, 75, 4525-4538.	3.0	63
93	Rotational distributions from photodissociations. IV. The bent triatomic molecule. Journal of Chemical Physics, 1983, 78, 6045-6065.	3.0	63
94	Application of complete space multireference manyâ€body perturbation theory to N2: Dependence on reference space andH0. Journal of Chemical Physics, 1995, 102, 1306-1333.	3.0	62
95	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
96	Huggins coefficient for the viscosity of polymer solutions. Journal of Chemical Physics, 1975, 62, 4032-4035.	3.0	61
97	Renormalization group and critical localization. Physical Review B, 1977, 15, 4476-4489.	3.2	61
98	Modification of the Phase Stability of Polymer Blends by Diblock Copolymer Additives. Macromolecules, 1995, 28, 2276-2287.	4.8	61
99	Lattice Cluster Theory for Pedestrians:Â The Incompressible Limit and the Miscibility of Polyolefin Blends. Macromolecules, 1998, 31, 6681-6690.	4.8	61
100	Lattice model of living polymerization. II. Interplay between polymerization and phase stability. Journal of Chemical Physics, 2000, 112, 1002-1010.	3.0	61
101	Influence of Cohesive Energy and Chain Stiffness on Polymer Glass Formation. Macromolecules, 2014, 47, 6990-6997.	4.8	61
102	Influence of Cohesive Energy on Relaxation in a Model Glass-Forming Polymer Melt. Macromolecules, 2016, 49, 8355-8370.	4.8	60
103	On scaling theories of polymer solutions. Journal of Chemical Physics, 1978, 69, 3647-3659.	3.0	59
104	Influence of blend compressibility on extrapolated zero-angle coherent scattering and spinodal: limitations of RPA [random-phase approximation] analysis. Macromolecules, 1990, 23, 1519-1526.	4.8	59
105	Lattice Cluster Theory of Multicomponent Polymer Systems: Chain Semiflexibility and Specific Interactions. Advances in Chemical Physics, 2007, , 335-390.	0.3	59
106	Mimicking the folding pathway to improve homology-free protein structure prediction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3734-3739.	7.1	59
107	Electron Localization in Disordered Systems. Physical Review B, 1972, 5, 4802-4826.	3.2	58
108	Modeling the Hydration Layer around Proteins: HyPred. Biophysical Journal, 2010, 99, 1611-1619.	0.5	57

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109	Random Matrix Theory and the Master Equation for Finite Systems. Journal of Chemical Physics, 1972, 57, 4699-4712.	3.0	56
110	Huggins Coefficient for Polymer Solutions with Excluded Volume. Macromolecules, 1977, 10, 899-906.	4.8	56
111	Role of monomer structure and compressibility on the properties of multicomponent polymer blends and solutions. Theoretica Chimica Acta, 1992, 82, 357-382.	0.8	56
112	Large-Scale Context in Protein Folding:Â Villin Headpieceâ€. Biochemistry, 2003, 42, 664-671.	2.5	56
113	Collision dyanamics of collision induced intersystem crossing processes. Chemical Physics, 1978, 33, 249-266.	1.9	55
114	Renormalization and the two-parameter theory. 2. Comparison with experiment and other two-parameter theories. Macromolecules, 1985, 18, 201-211.	4.8	55
115	Convergence behavior of multireference perturbation theory: Forced degeneracy and optimization partitioning applied to the beryllium atom. Physical Review A, 1996, 54, 343-356.	2.5	55
116	Crowding Induced Self-Assembly and Enthalpy-Entropy Compensation. Physical Review Letters, 2009, 103, 135701.	7.8	55
117	Influence of nonlinear electrostatics on transfer energies between liquid phases: Charge burial is far less expensive than Born model. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 11146-11151.	7.1	54
118	Valence Excited States of BeO. Journal of Chemical Physics, 1967, 46, 3556-3565.	3.0	53
119	Quantum theory of photodissociation of polyatomic molecules: Application to HCN. Chemical Physics Letters, 1974, 28, 328-334.	2.6	53
120	Lattice theory of polymer blends and liquid mixtures: Beyond the Floryâ€“Huggins approximation. Journal of Chemical Physics, 1989, 90, 2017-2026.	3.0	53
121	Photodissociation of Diatomic Molecules to Open Shell Atoms. Advances in Chemical Physics, 2007, , 1-113.	0.3	53
122	Considerations on the Rotationâ€"Vibration of Triatomic Molecules. Journal of Chemical Physics, 1966, 45, 591-598.	3.0	52
123	Direct first principles algorithm for the universal electron density functional. Journal of Chemical Physics, 1982, 77, 396-398.	3.0	52
124	Nuclear coordinate dependence of electronic matrix elements for radiationless transitions. Chemical Physics, 1975, 11, 409-432.	1.9	51
125	Langevin-Debye Model for Nonlinear Electrostatic Screening of Solvated Ions. Physical Review Letters, 2009, 102, 057603.	7.8	51
126	Entropyâ^'Enthalpy Compensation in Chemical Reactions and Adsorption: An Exactly Solvable Model. Journal of Physical Chemistry B, 2011, 115, 1689-1692.	2.6	51

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127	Theory of collision induced intersystem crossing. Application to glyoxal. Chemical Physics Letters, 1976, 37, 47-50.	2.6	50
128	Dynamics of electronic dephasing in the Fennaâ€“Matthewsâ€“Olson complex. New Journal of Physics, 2010, 12, 065042.	2.9	50
129	Diffusion controlled processes among stationary reactive sinks: Effective medium approach. Journal of Chemical Physics, 1983, 78, 2573-2578.	3.0	49
130	Dense self-interacting lattice trees with specified topologies: From light to dense branching. Physical Review A, 1992, 45, 7111-7127.	2.5	49
131	How far is far from critical point in polymer blends? Lattice cluster theory computations for structured monomer, compressible systems. Journal of Chemical Physics, 1993, 99, 4804-4820.	3.0	47
132	Solvation effect on conformations of 1,2:dimethoxyethane: Charge-dependent nonlinear response in implicit solvent models. Journal of Chemical Physics, 2008, 128, 034501.	3.0	47
133	Renormalization group treatment of polymer excluded volume by tâ€™Hooftâ€“Veltmanâ€type dimensional regularization. Journal of Chemical Physics, 1983, 78, 7390-7411.	3.0	46
134	Global threeâ€dimensional potential energy surfaces of H2S from the ab initio effective valence shell Hamiltonian method. Journal of Chemical Physics, 1996, 105, 8754-8768.	3.0	46
135	A study of the rotational state dependence of predissociation of a polyatomic molecule: The case of ClO2. Journal of Chemical Physics, 1981, 74, 3089-3101.	3.0	45
136	Static-coherent-scattering function for a single polymer chain: Conformational space renormalization of polymers. V. Physical Review A, 1982, 25, 2801-2811.	2.5	45
137	Lattice models of polymer fluids: Monomers occupying several lattice sites. II. Interaction energies. Journal of Chemical Physics, 1989, 90, 2003-2016.	3.0	45
138	On the large entropic contribution to the effective interaction parameter of polystyreneâ€“poly(methyl) Tj ETQq0 0 0 rgBT /Overlock 10	3.0	45
139	Competition between Hydrodynamic Screening ("Draining") and Excluded Volume Interactions in an Isolated Polymer Chain. Macromolecules, 1994, 27, 6088-6099.	4.8	45
140	Thermodynamic regulation of actin polymerization. Journal of Chemical Physics, 2001, 114, 10573-10576.	3.0	45
141	Direct computation of characteristic temperatures and relaxation times for glass-forming polymer liquids. Journal of Chemical Physics, 2005, 123, 111102.	3.0	45
142	Shake-up peak positions and intensities by many-body theory methods. Chemical Physics, 1978, 32, 437-449.	1.9	44
143	A one-dimensional microscopic model for thermal desorption of an atom. Applications to the case of weak binding. Chemical Physics Letters, 1980, 74, 43-48.	2.6	44
144	Excited potential energy surfaces of CH3SH from the ab initio effective valence shell Hamiltonian method. Journal of Chemical Physics, 1994, 101, 4832-4841.	3.0	44

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145	Potential energy curve for isomerization of N2H2 and C2H4 using the improved virtual orbital multireference MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2008, 128, 144304.	3.0	44
146	De novo prediction of protein folding pathways and structure using the principle of sequential stabilization. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17442-17447.	7.1	44
147	Molecular Origins of Cofilin-Linked Changes in Actin Filament Mechanics. Journal of Molecular Biology, 2013, 425, 1225-1240.	4.2	44
148	Dynamics and spectroscopy of near threshold nonadiabatic resonances in photodissociation to open shell atoms: CH+a model system. Journal of Chemical Physics, 1986, 85, 2699-2717.	3.0	43
149	Comparison of the perturbative convergence with multireference MÃ¶llerâ€“Plesset, Epsteinâ€“Nesbet, forced degenerate and optimized zeroth order partitionings: The excited BeH2surface. Journal of Chemical Physics, 1997, 106, 4067-4081.	3.0	43
150	Beyond Flory-Huggins Theory: New Classes of Blend Miscibility Associated with Monomer Structural Asymmetry. Physical Review Letters, 2002, 88, 095503.	7.8	43
151	Conformation space renormalization of polymers. I. Single chain equilibrium properties using Wilsonâ€type renormalization. Journal of Chemical Physics, 1981, 75, 993-1008.	3.0	42
152	Polypeptide dynamics: Experimental tests of an optimized Rouseâ€“Zimm type model. Journal of Chemical Physics, 1990, 93, 822-836.	3.0	42
153	Static structure factors of compressible polymer blends and diblock copolymer melts. 2. Constraints on density fluctuations. Macromolecules, 1991, 24, 958-966.	4.8	42
154	Polymer melt near a solid wall. Journal of Chemical Physics, 1994, 101, 9143-9154.	3.0	42
155	Intramolecular vibrational relaxation: electronic relaxation as a probe. Chemical Physics Letters, 1976, 42, 600-606.	2.6	41
156	Microscopic theory of polymer internal viscosity: Mode coupling approximation for the Rouse model. Journal of Chemical Physics, 1977, 67, 1380-1393.	3.0	41
157	Influence of monomer molecular structure on the glass transition in polymers I. Lattice cluster theory for the configurational entropy. Journal of Chemical Physics, 2003, 119, 5730-5739.	3.0	41
158	Ab initio third order effective valence shell Hamiltonian calculations for first row diatomic hydrides. Journal of Chemical Physics, 1981, 74, 6842-6848.	3.0	40
159	The polymerization of actin: Thermodynamics near the polymerization line. Journal of Chemical Physics, 2003, 119, 4070-4084.	3.0	40
160	Minimalist Representations and the Importance of Nearest Neighbor Effects in Protein Folding Simulations. Journal of Molecular Biology, 2006, 363, 835-857.	4.2	40
161	Communication: Towards first principles theory of relaxation in supercooled liquids formulated in terms of cooperative motion. Journal of Chemical Physics, 2014, 141, 141102.	3.0	40
162	The meaning of the â€œuniversalâ€•WLF parameters of glass-forming polymer liquids. Journal of Chemical Physics, 2015, 142, 014905.	3.0	40

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163	Critical analysis of equations-of-motionâ€”Green's function method: Ionization potentials of N2. Chemical Physics Letters, 1977, 46, 1-7.	2.6	39
164	A lattice model for selfâ€•and mutually avoiding semiflexible polymer chains. Journal of Chemical Physics, 1987, 86, 3720-3730.	3.0	39
165	Dipole moments, transition moments, oscillator strengths, radiative lifetimes, and overtone intensities for CH and CH+ as computed by quasi-degenerate many-body perturbation theory. International Journal of Quantum Chemistry, 1991, 39, 269-286.	2.0	39
166	Tests and Applications of Complete Model Space Quasidegenerate Many-Body Perturbation Theory for Molecules. Lecture Notes in Quantum Chemistry II, 1989, , 1-21.	0.3	39
167	Large isotope effects in photodissociation of polyatomic molecules. Journal of Chemical Physics, 1975, 63, 4479-4484.	3.0	38
168	Generalized perturbation theory of effective valence shell hamiltonians. Chemical Physics Letters, 1979, 61, 577-582.	2.6	38
169	Angular distributions from photodissociations. V. The bent triatomic molecule. Journal of Chemical Physics, 1983, 78, 6066-6078.	3.0	38
170	Influence of Monomer Structure and Interaction Asymmetries on the Miscibility and Interfacial Properties of Polyolefin Blends. Macromolecules, 1996, 29, 8960-8972.	4.8	38
171	Collision-Induced Intersystem Crossing. Advances in Chemical Physics, 2007, , 291-336.	0.3	38
172	Energy distribution in selected fragment vibrations in dissociation processes in polyatomic molecules. Journal of Chemical Physics, 1977, 67, 1462-1472.	3.0	37
173	Rotational mechanism for vibrational relaxation in rigid media. Interaction potentials. Chemical Physics Letters, 1977, 49, 19-23.	2.6	37
174	Elastic properties of a polymer chain with excluded volume: a renormalization group theory. Macromolecules, 1981, 14, 880-881.	4.8	37
175	Excluded volume effects for polymers in presence of interacting surfaces: Chain conformation renormalization group. Journal of Chemical Physics, 1985, 83, 4166-4182.	3.0	37
176	Polymer-polymer and polymer-surface excluded volume effects in flexible polymers attached to an interface: comparison of renormalization group calculations with Monte Carlo and direct enumeration data. Macromolecules, 1986, 19, 2041-2054.	4.8	37
177	Abinitiostudy of cyclobutadiene using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 1993, 99, 7833-7844.	3.0	37
178	New patterns of polymer blend miscibility associated with monomer shape and size asymmetry. Journal of Chemical Physics, 2002, 116, 9983-9996.	3.0	37
179	Collisional Effects on Electronic Relaxation Processes. Advances in Chemical Physics, 2007, , 207-269.	0.3	37
180	Reduced C_{Î²} statistical potentials can outperform allâ€atom potentials in decoy identification. Protein Science, 2007, 16, 2123-2139.	7.6	37

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181	Pressure dependence of electronic relaxation: A stochastic model. Journal of Chemical Physics, 1974, 61, 3942-3953.	3.0	36
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