James L Skinner

List of Publications by Year in descending order

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LAMES | SKINNED

#	Article	IF	CITATIONS
1	IR Spectroscopy Can Reveal the Mechanism of K+ Transport in Ion Channels. Biophysical Journal, 2020, 118, 254-261.	0.2	17
2	Controlling the Structure of MoS ₂ Membranes via Covalent Functionalization with Molecular Spacers. Nano Letters, 2020, 20, 7844-7851.	4.5	34
3	Unusually strong hydrogen bond cooperativity in particular (H ₂ 0) ₂₀ clusters. Physical Chemistry Chemical Physics, 2020, 22, 18124-18131.	1.3	24
4	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	23.0	205
5	Dephasing and Decoherence in Vibrational and Electronic Line Shapes. Journal of Physical Chemistry B, 2020, 124, 1531-1542.	1.2	5
6	Machine Learning for Vibrational Spectroscopic Maps. Journal of Chemical Theory and Computation, 2019, 15, 6850-6858.	2.3	49
7	OH-Stretch Raman Multivariate Curve Resolution Spectroscopy of HOD/H2O Mixtures. Journal of Physical Chemistry B, 2019, 123, 5139-5146.	1.2	10
8	Mid-IR spectroscopy of supercritical water: From dilute gas to dense fluid. Journal of Chemical Physics, 2019, 150, 054505.	1.2	11
9	Second-Order Vibrational Lineshapes from the Air/Water Interface. Journal of Physical Chemistry A, 2018, 122, 4457-4464.	1.1	63
10	Perspective: Crossing the Widom line in no man's land: Experiments, simulations, and the location of the liquid-liquid critical point in supercooled water. Journal of Chemical Physics, 2018, 149, 140901.	1.2	69
11	Percolation in supercritical water: Do the Widom and percolation lines coincide?. Journal of Chemical Physics, 2018, 149, 084504.	1.2	23
12	Communication: Diffusion constant in supercooled water as the Widom line is crossed in no man's land. Journal of Chemical Physics, 2018, 148, 191102.	1.2	13
13	Fermi resonance in OH-stretch vibrational spectroscopy of liquid water and the water hexamer. Journal of Chemical Physics, 2018, 148, 244107.	1.2	64
14	Super-Maxwellian helium evaporation from pure and salty water. Journal of Chemical Physics, 2016, 144, 044707.	1.2	15
15	Low-frequency dynamics of aqueous alkali chloride solutions as probed by terahertz spectroscopy. Journal of Chemical Physics, 2016, 144, 234501.	1.2	12
16	Communication: Vibrational sum-frequency spectrum of the air-water interface, revisited. Journal of Chemical Physics, 2016, 145, 031103.	1.2	58
17	IR spectra of water droplets in no man's land and the location of the liquid-liquid critical point. Journal of Chemical Physics, 2016, 145, 124509.	1.2	22
18	Instantaneous ion configurations in the K ⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. Science, 2016, 353, 1040-1044.	6.0	174

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19	Sub- and super-Maxwellian evaporation of simple gases from liquid water. Journal of Chemical Physics, 2016, 144, 154701.	1.2	8
20	Evidence for a liquid-liquid critical point in supercooled water within the E3B3 model and a possible interpretation of the kink in the homogeneous nucleation line. Journal of Chemical Physics, 2016, 144, 214501.	1.2	65
21	Two-dimensional infrared spectroscopy of neat ice I _h . Physical Chemistry Chemical Physics, 2016, 18, 3772-3779.	1.3	26
22	Water Dynamics in Gyroid Phases of Self-Assembled Gemini Surfactants. Journal of the American Chemical Society, 2016, 138, 2472-2475.	6.6	34
23	IR and SFG vibrational spectroscopy of the water bend in the bulk liquid and at the liquid-vapor interface, respectively. Journal of Chemical Physics, 2015, 143, 014502.	1.2	81
24	Mixed quantum/classical approach to OH-stretch inelastic incoherent neutron scattering spectroscopy for ambient and supercooled liquid water and ice Ih. Journal of Chemical Physics, 2015, 143, 014503.	1.2	3
25	Reparametrized E3B (Explicit Three-Body) Water Model Using the TIP4P/2005 Model as a Reference. Journal of Chemical Theory and Computation, 2015, 11, 2268-2277.	2.3	43
26	Theoretical Sum Frequency Generation Spectroscopy of Peptides. Journal of Physical Chemistry B, 2015, 119, 8969-8983.	1.2	25
27	Assessment of amide I spectroscopic maps for a gas-phase peptide using IR-UV double-resonance spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2014, 140, 224111.	1.2	26
28	Ultrafast pump-probe and 2DIR anisotropy and temperature-dependent dynamics of liquid water within the E3B model. Journal of Chemical Physics, 2014, 141, 024509.	1.2	16
29	Theoretical vibrational sum-frequency generation spectroscopy of water near lipid and surfactant monolayer interfaces. II. Two-dimensional spectra. Journal of Chemical Physics, 2014, 141, 22D505.	1.2	34
30	A scaled-ionic-charge simulation model that reproduces enhanced and suppressed water diffusion in aqueous salt solutions. Journal of Chemical Physics, 2014, 141, 104507.	1.2	109
31	Structural motif of polyglutamine amyloid fibrils discerned with mixed-isotope infrared spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5796-5801.	3.3	105
32	Resonant vibrational energy transfer in ice Ih. Journal of Chemical Physics, 2014, 140, 244503.	1.2	8
33	Dielectric constant and low-frequency infrared spectra for liquid water and ice Ih within the E3B model. Journal of Chemical Physics, 2014, 141, 084508.	1.2	25
34	Theoretical vibrational sum-frequency generation spectroscopy of water near lipid and surfactant monolayer interfaces. Journal of Chemical Physics, 2014, 141, 18C502.	1.2	57
35	Structure and OH-stretch spectroscopy of low- and high-density amorphous ices. Journal of Chemical Physics, 2014, 140, 134503.	1.2	32
36	Dynamics of Water Confined in Reversed Micelles: Multidimensional Vibrational Spectroscopy Study. Journal of Physical Chemistry B, 2013, 117, 15545-15558.	1.2	82

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37	Hydrogen Bonding and OH-Stretch Spectroscopy in Water: Hexamer (Cage), Liquid Surface, Liquid, and Ice. Journal of Physical Chemistry Letters, 2013, 4, 12-17.	2.1	87
38	Robustness of Frequency, Transition Dipole, and Coupling Maps for Water Vibrational Spectroscopy. Journal of Chemical Theory and Computation, 2013, 9, 3109-3117.	2.3	86
39	Proton Disorder in Ice Ih and Inhomogeneous Broadening in Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 15536-15544.	1.2	20
40	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. III. Water clustering and vibrational energy transfer. Journal of Chemical Physics, 2013, 139, 175103.	1.2	12
41	Slow hydrogen-bond switching dynamics at the water surface revealed by theoretical two-dimensional sum-frequency spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1992-1998.	3.3	88
42	The water hexamer: Three-body interactions, structures, energetics, and OH-stretch spectroscopy at finite temperature. Journal of Chemical Physics, 2012, 137, 104304.	1.2	85
43	Vibrational Spectroscopy of Water at Interfaces. Accounts of Chemical Research, 2012, 45, 93-100.	7.6	123
44	Parallel Î ² -Sheet Vibrational Couplings Revealed by 2D IR Spectroscopy of an Isotopically Labeled Macrocycle: Quantitative Benchmark for the Interpretation of Amyloid and Protein Infrared Spectra. Journal of the American Chemical Society, 2012, 134, 19118-19128.	6.6	91
45	Interpretation of IR and Raman Line Shapes for H ₂ O and D ₂ O Ice Ih. Journal of Physical Chemistry B, 2012, 116, 13821-13830.	1.2	92
46	2DIR Spectroscopy of Human Amylin Fibrils Reflects Stable β-Sheet Structure. Journal of the American Chemical Society, 2011, 133, 16062-16071.	6.6	114
47	Collective Hydrogen Bond Reorganization in Water Studied with Temperature-Dependent Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry B, 2011, 115, 5604-5616.	1.2	92
48	Development and Validation of Transferable Amide I Vibrational Frequency Maps for Peptides. Journal of Physical Chemistry B, 2011, 115, 3713-3724.	1.2	162
49	Surface of Liquid Water: Three-Body Interactions and Vibrational Sum-Frequency Spectroscopy. Journal of the American Chemical Society, 2011, 133, 10360-10363.	6.6	103
50	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. I. Infrared spectra and ultrafast pump-probe observables. Journal of Chemical Physics, 2011, 135, 075101.	1.2	50
51	Interpretation of the water surface vibrational sum-frequency spectrum. Journal of Chemical Physics, 2011, 135, 044701.	1.2	118
52	Hydrogen bonding at the water surface revealed by isotopic dilution spectroscopy. Nature, 2011, 474, 192-195.	13.7	380
53	Vibrational energy relaxation of small molecules and ions in liquids. Theoretical Chemistry Accounts, 2011, 128, 147-155.	0.5	32
54	Time-averaging approximation in the interaction picture: Absorption line shapes for coupled chromophores with application to liquid water. Journal of Chemical Physics, 2011, 135, 154114.	1.2	13

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55	Vibrational spectroscopy of water in hydrated lipid multi-bilayers. II. Two-dimensional infrared and peak shift observables within different theoretical approximations. Journal of Chemical Physics, 2011, 135, 164506.	1.2	26
56	Robust three-body water simulation model. Journal of Chemical Physics, 2011, 134, 184501.	1.2	115
57	Infrared and Raman line shapes for ice Ih. I. Dilute HOD in H2O and D2O. Journal of Chemical Physics, 2010, 132, 204505.	1.2	88
58	Following the Motions of Water Molecules in Aqueous Solutions. Science, 2010, 328, 985-986.	6.0	45
59	Two-dimensional infrared spectroscopy and ultrafast anisotropy decay of water. Journal of Chemical Physics, 2010, 132, 224503.	1.2	101
60	Vibrational Spectroscopy as a Probe of Structure and Dynamics in Liquid Water. Chemical Reviews, 2010, 110, 1498-1517.	23.0	640
61	2D IR Line Shapes Probe Ovispirin Peptide Conformation and Depth in Lipid Bilayers. Journal of the American Chemical Society, 2010, 132, 2832-2838.	6.6	90
62	Signatures of coherent vibrational energy transfer in IR and Raman line shapes for liquid water. Physical Chemistry Chemical Physics, 2010, 12, 982-991.	1.3	93
63	Infrared and Raman line shapes for ice Ih. II. H2O and D2O. Journal of Chemical Physics, 2010, 133, 244504.	1.2	85
64	Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions. Journal of Chemical Physics, 2009, 131, 144511.	1.2	135
65	Gating Mechanism of the Influenza A M2 Channel Revealed by 1D and 2D IR Spectroscopies. Structure, 2009, 17, 247-254.	1.6	116
66	Vibrational Sum-Frequency Spectroscopy of the Water Liquid/Vapor Interface. Journal of Physical Chemistry B, 2009, 113, 4125-4130.	1.2	102
67	Empirical Amide I Vibrational Frequency Map: Application to 2D-IR Line Shapes for Isotope-Edited Membrane Peptide Bundles. Journal of Physical Chemistry B, 2009, 113, 592-602.	1.2	129
68	Vibrational Spectroscopy and Dynamics of Water Confined inside Reverse Micelles. Journal of Physical Chemistry B, 2009, 113, 15017-15028.	1.2	134
69	IR and Raman spectra of liquid water: Theory and interpretation. Journal of Chemical Physics, 2008, 128, 224511.	1.2	490
70	Water Simulation Model with Explicit Three-Molecule Interactions. Journal of Physical Chemistry B, 2008, 112, 8311-8318.	1.2	100
71	Vibrational sum-frequency spectroscopy of the liquid/vapor interface for dilute HOD in D2O. Journal of Chemical Physics, 2008, 129, 214705.	1.2	95
72	Hydrogen bonding and Raman, IR, and 2D-IR spectroscopy of dilute HOD in liquid D2O. Proceedings of the United States of America, 2007, 104, 14215-14220.	3.3	346

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73	Dynamical effects in line shapes for coupled chromophores: Time-averaging approximation. Journal of Chemical Physics, 2007, 127, 104105.	1.2	88
74	Optical Dephasing of Ions and Molecules in Crystals. Advances in Chemical Physics, 2007, , 1-44.	0.3	46
75	Hydrogen bonding definitions and dynamics in liquid water. Journal of Chemical Physics, 2007, 126, 204107.	1.2	576
76	Approaches for the calculation of vibrational frequencies in liquids: Comparison to benchmarks for azide/water clusters. Journal of Chemical Physics, 2006, 124, 204110.	1.2	66
77	Pronounced non-Condon effects in the ultrafast infrared spectroscopy of water. Journal of Chemical Physics, 2005, 123, 044513.	1.2	257
78	Quantum corrections in vibrational and electronic condensed phase spectroscopy: Line shapes and echoes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6720-6725.	3.3	42
79	A Mode-Coupling Theory of Vibrational Line Broadening in Near-Critical Fluidsâ€. Journal of Physical Chemistry B, 2005, 109, 6879-6883.	1.2	6
80	Infrared and Raman Line Shapes of Dilute HOD in Liquid H2O and D2O from 10 to 90 °C. Journal of Physical Chemistry A, 2005, 109, 6154-6165.	1.1	298
81	Combined electronic structure/molecular dynamics approach for ultrafast infrared spectroscopy of dilute HOD in liquid H2O and D2O. Journal of Chemical Physics, 2004, 120, 8107-8117.	1.2	330
82	Quantum dynamics in simple fluids. Journal of Chemical Physics, 2004, 120, 6621-6624.	1.2	53
83	Dynamics of water probed with vibrational echo correlation spectroscopy. Journal of Chemical Physics, 2004, 121, 12431.	1.2	337
84	Spectral diffusion in a fluctuating charge model of water. Journal of Chemical Physics, 2004, 121, 8897-8900.	1.2	90
85	Ultrafast vibrational spectroscopy of water and aqueous N-methylacetamide: Comparison of different electronic structure/molecular dynamics approaches. Journal of Chemical Physics, 2004, 121, 8887-8896.	1.2	243
86	Water Dynamics:  Vibrational Echo Correlation Spectroscopy and Comparison to Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2004, 108, 1107-1119.	1.1	436
87	Vibrational spectroscopy of HOD in liquid D2O. III. Spectral diffusion, and hydrogen-bonding and rotational dynamics. Journal of Chemical Physics, 2003, 118, 264-272.	1.2	375
88	Liquid state theories for the structure of water. Journal of Chemical Physics, 2003, 119, 13012-13016.	1.2	29
89	Hydrodynamic boundary conditions, the Stokes–Einstein law, and long-time tails in the Brownian limit. Journal of Chemical Physics, 2003, 119, 8062-8068.	1.2	112
90	Vibrational spectroscopy of HOD in liquid D2O. VI. Intramolecular and intermolecular vibrational energy flow. Journal of Chemical Physics, 2003, 119, 1623-1633.	1.2	100

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91	Vibrational spectroscopy of HOD in liquid D2O. VII. Temperature and frequency dependence of the OH stretch lifetime. Journal of Chemical Physics, 2003, 119, 3840-3848.	1.2	62
92	Vibrational spectroscopy of HOD in liquid D2O. V. Infrared three-pulse photon echoes. Journal of Chemical Physics, 2003, 118, 9672-9679.	1.2	74
93	Vibrational spectroscopy of HOD in liquid D2O. IV. Infrared two-pulse photon echoes. Journal of Chemical Physics, 2003, 118, 9664-9671.	1.2	56
94	Vibrational spectroscopy of HOD in liquid D2O. I. Vibrational energy relaxation. Journal of Chemical Physics, 2002, 117, 5827-5838.	1.2	154
95	Vibrational spectroscopy of HOD in liquid D2O. II. Infrared line shapes and vibrational Stokes shift. Journal of Chemical Physics, 2002, 117, 8847-8854.	1.2	183
96	Calculating Vibrational Energy Relaxation Rates from Classical Molecular Dynamics Simulations:Â Quantum Correction Factors for Processes Involving Vibrationâ°'Vibration Energy Transferâ€. Journal of Physical Chemistry B, 2001, 105, 6716-6721.	1.2	93
97	Determining the solvation correlation function from three-pulse photon echoes in liquids. Journal of Chemical Physics, 2001, 114, 1326-1335.	1.2	68
98	Isotropic Raman line shapes of N2 and O2 along their liquid–gas coexistence lines. Journal of Chemical Physics, 2001, 115, 8531-8539.	1.2	29
99	Vibrational energy relaxation of polyatomic solutes in simple liquids and supercritical fluids. Journal of Chemical Physics, 2000, 112, 275-281.	1.2	77
100	Vibrational Line Shifts in Supercritical Fluids. Journal of Physical Chemistry A, 2000, 104, 483-489.	1.1	28
101	Vibrational energy relaxation of oxygen in liquid mixtures with argon. Journal of Chemical Physics, 1999, 110, 4467-4470.	1.2	46
102	Quantum Dynamics and Vibrational Relaxation. Journal of Physical Chemistry A, 1999, 103, 9494-9499.	1.1	202
103	Spectral Diffusion in Proteins:  A Simple Phenomenological Model. Journal of Physical Chemistry A, 1999, 103, 2310-2311.	1.1	19
104	Argon Scattering off the Surface of Liquid Indium:Â Exit Angle and Energy Dependence. Journal of Physical Chemistry B, 1998, 102, 206-211.	1.2	31
105	Two-pulse photon echoes from zinc-meso-tetraphenylporphine/polymethylmethacrylate are not consistent with the tunneling two-level system model. Journal of Chemical Physics, 1998, 108, 8485-8488.	1.2	7
106	Optical line shapes of single molecules in glasses: Temperature and scan-time dependence. Journal of Chemical Physics, 1998, 109, 4920-4926.	1.2	24
107	Absorption line shapes and solvation dynamics of CH3I in supercritical Ar. Journal of Chemical Physics, 1997, 107, 10485-10491.	1.2	35
108	Semiclassical approximations to golden rule rate constants. Journal of Chemical Physics, 1997, 107, 8717-8718.	1.2	54

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109	Vibrational energy relaxation of diatomic molecules in rare gas crystals. Journal of Chemical Physics, 1997, 106, 1034-1040.	1.2	31
110	Molecular theory of electronic spectroscopy in nonpolar fluids: Ultrafast solvation dynamics and absorption and emission line shapes. Journal of Chemical Physics, 1997, 106, 2129-2144.	1.2	151
111	Theory of photon echoes and hole burning in low temperature glasses: How good are the standard approximations?. Journal of Chemical Physics, 1997, 107, 7630-7641.	1.2	36
112	On the Distribution of Single Molecule Line Widths in Low-Temperature Glasses. Molecular Crystals and Liquid Crystals, 1996, 291, 73-80.	0.3	4
113	A theory of vibrational energy relaxation in liquids. Journal of Chemical Physics, 1996, 105, 7047-7058.	1.2	162
114	An improved theory of multiphonon relaxation in solids. Journal of Chemical Physics, 1996, 105, 10153-10155.	1.2	33
115	Spectral Dynamics of Individual Molecules in Solids. Molecular Crystals and Liquid Crystals, 1996, 283, 89-93.	0.3	0
116	Spectral diffusion of individual pentacene molecules inPâ€ŧerphenyl crystal: Stochastic theoretical model and analysis of experimental data. Journal of Chemical Physics, 1995, 102, 1540-1552.	1.2	78
117	On the relaxation of a twoâ€level system driven by a strong electromagnetic field. Journal of Chemical Physics, 1995, 102, 8541-8561.	1.2	119
118	On the theory of multiphonon relaxation rates in solids. Journal of Chemical Physics, 1995, 103, 1533-1543.	1.2	78
119	On the ratio T2/T1 for nonâ€Ohmic spectral densities. Journal of Chemical Physics, 1994, 101, 852-852.	1.2	3
120	Spectroscopy of a chromophore coupled to a lattice of dynamic twoâ€level systems. II. Spectral diffusion kernel. Journal of Chemical Physics, 1994, 101, 965-973.	1.2	41
121	Spectroscopy of a chromophore coupled to a lattice of dynamic twoâ€level systems. I. Absorption line shape. Journal of Chemical Physics, 1994, 101, 959-964.	1.2	58
122	A molecular theory of the line shape: Inhomogeneous and homogeneous electronic spectra of dilute chromophores in nonpolar fluids. Journal of Chemical Physics, 1993, 99, 4391-4402.	1.2	146
123	Molecular theory of transition energy correlations for pairs of chromophores in liquids or glasses. Journal of Chemical Physics, 1992, 97, 8-18.	1.2	30
124	T2 can be greater than 2T1 even at finite temperature. Journal of Chemical Physics, 1991, 94, 4405-4410.	1.2	56
125	Quantumâ€mechanical derivation of the Bloch equations: Beyond the weakâ€coupling limit. Journal of Chemical Physics, 1991, 94, 4391-4404.	1.2	141
126	Single-molecule probes. Nature, 1991, 349, 195-195.	13.7	2

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127	Classical and quantum continuum percolation with hard core interactions. Journal of Chemical Physics, 1991, 94, 6153-6159.	1.2	13
128	Critical exponents for Anderson localization. Journal of Chemical Physics, 1990, 93, 8973-8982.	1.2	47
129	T2can be greater than 2T1. Journal of Chemical Physics, 1989, 91, 1775-1782.	1.2	39
130	On the microscopic nature of inhomogeneously broadened spectra of chromophores in glasses and crystals. Journal of Chemical Physics, 1989, 90, 3880-3881.	1.2	40
131	Microscopic theory of reversible pressure broadening in holeâ€burning spectra of impurities in glasses. Journal of Chemical Physics, 1989, 90, 3274-3281.	1.2	156
132	Renormalizationâ€group approach to the metal–insulator transition in doped semiconductors. Journal of Chemical Physics, 1989, 90, 2703-2707.	1.2	4
133	Localization phase diagram for the energetically and substitutionally disordered Anderson/quantum percolation model. Journal of Chemical Physics, 1988, 89, 3279-3284.	1.2	52
134	Nonperturbative theory of temperatureâ€dependent optical dephasing in crystals. IV. Microscopic model for pseudolocal phonons. Journal of Chemical Physics, 1987, 87, 54-59.	1.2	20
135	Nonperturbative theory of temperatureâ€dependent optical dephasing in crystals. II. Pseudolocal phonons. Journal of Chemical Physics, 1985, 83, 2097-2106.	1.2	64
136	Nonperturbative theory of temperatureâ€dependent optical dephasing in crystals. III. Comparison with experiment. Journal of Chemical Physics, 1985, 83, 2107-2115.	1.2	45
137	Exciton dynamics and transient grating experiments. Journal of Chemical Physics, 1985, 82, 260-269.	1.2	37
138	Kinetic Ising model for polymer dynamics. II. Generalized transition rates and the Williams–Watts nonexponential function. Journal of Chemical Physics, 1985, 82, 5232-5241.	1.2	41
139	Nonperturbative theory of temperatureâ€dependent optical dephasing in crystals. I. Acoustic or optical phonons. Journal of Chemical Physics, 1984, 81, 5471-5479.	1.2	81
140	Optical dephasing and photon echoes from energetically and substitutionally disordered crystals. Journal of Chemical Physics, 1984, 81, 5310-5318.	1.2	36
141	On the thermal broadening of zeroâ€phonon impurity lines in absorption and fluorescence spectra. Journal of Chemical Physics, 1984, 81, 1604-1613.	1.2	106
142	Kinetic Ising model for polymer dynamics: Applications to dielectric relaxation and dynamic depolarized light scattering. Journal of Chemical Physics, 1983, 79, 1955-1964.	1.2	90
143	The theory of photon echoes for strongly coupled electron–phonon systems. Journal of Chemical Physics, 1982, 77, 3398-3405.	1.2	28