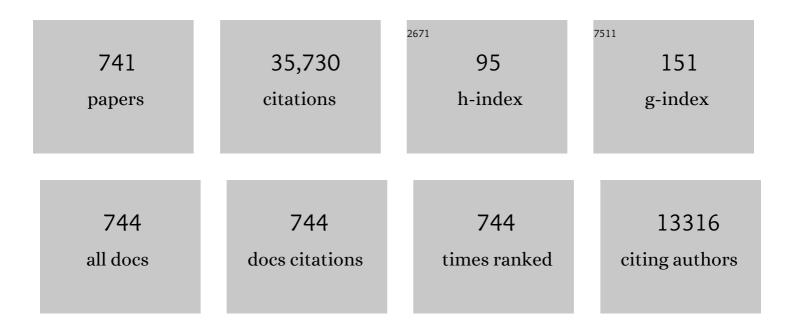
Shaul Mukamel

List of Publications by Year in descending order

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#	Article	lF	CITATIONS
1	Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems. Reviews of Modern Physics, 2009, 81, 1665-1702.	16.4	1,067
2	MULTIDIMENSIONALFEMTOSECONDCORRELATIONSPECTROSCOPIES OFELECTRONIC ANDVIBRATIONALEXCITATIONS. Annual Review of Physical Chemistry, 2000, 51, 691-729.	4.8	796
3	Twoâ€dimensional femtosecond vibrational spectroscopy of liquids. Journal of Chemical Physics, 1993, 99, 9496-9511.	1.2	559
4	Density Matrix Analysis and Simulation of Electronic Excitations in Conjugated and Aggregated Molecules. Chemical Reviews, 2002, 102, 3171-3212.	23.0	519
5	Using coherence to enhance function in chemical and biophysical systems. Nature, 2017, 543, 647-656.	13.7	477
6	Coherent Multidimensional Optical Spectroscopy of Excitons in Molecular Aggregates; Quasiparticle versus Supermolecule Perspectives. Chemical Reviews, 2009, 109, 2350-2408.	23.0	446
7	Exciton-migration and three-pulse femtosecond optical spectroscopies of photosynthetic antenna complexes. Journal of Chemical Physics, 1998, 108, 7763-7774.	1.2	380
8	Electronic Coherence and Collective Optical Excitations of Conjugated Molecules. Science, 1997, 277, 781-787.	6.0	345
9	Experimental Determination of the Quantum-Mechanical State of a Molecular Vibrational Mode Using Fluorescence Tomography. Physical Review Letters, 1995, 74, 884-887.	2.9	294
10	Nonlinear susceptibilities of molecular aggregates: Enhancement ofχ(3)by size. Physical Review A, 1989, 40, 5783-5801.	1.0	270
11	Superradiance in molecular aggregates. Journal of Chemical Physics, 1989, 91, 683-700.	1.2	260
12	Femtosecond Optical Spectroscopy: A Direct Look at Elementary Chemical Events. Annual Review of Physical Chemistry, 1990, 41, 647-681.	4.8	257
13	Many-Body Approaches for Simulating Coherent Nonlinear Spectroscopies of Electronic and Vibrational Excitons. Chemical Reviews, 2004, 104, 2073-2098.	23.0	256
14	Dielectric friction and the transition from adiabatic to nonadiabatic electron transfer. I. Solvation dynamics in Liouville space. Journal of Chemical Physics, 1988, 88, 3263-3280.	1.2	250
15	Collisionless Multiphoton Dissociation of SF6: A Statistical Thermodynamic Process. Physical Review Letters, 1977, 38, 1131-1134.	2.9	249
16	Offâ€resonant transient birefringence in liquids. Journal of Chemical Physics, 1993, 99, 2410-2428.	1.2	248
17	Roadmap of ultrafast x-ray atomic and molecular physics. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 032003.	0.6	240
18	Photosynthetic reaction center as a quantum heat engine. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 2746-2751	3.3	234

#	Article	IF	CITATIONS
19	Nonlinear optical signals and spectroscopy with quantum light. Reviews of Modern Physics, 2016, 88, .	16.4	234
20	Quantum Extension of the Jarzynski Relation: Analogy with Stochastic Dephasing. Physical Review Letters, 2003, 90, 170604.	2.9	233
21	Femtosecond pump-probe spectroscopy of polyatomic molecules in condensed phases. Physical Review A, 1990, 41, 6485-6504.	1.0	224
22	Energy gap law for vibrational relaxation of a molecule in a dense medium. Journal of Chemical Physics, 1975, 63, 200-207.	1.2	221
23	Nonlinear optics of semiconductor and molecular nanostructures; a common perspective. Reviews of Modern Physics, 1998, 70, 145-174.	16.4	221
24	Some features of vibrational relaxation of a diatomic molecule in a dense medium. Journal of Chemical Physics, 1974, 60, 3929-3934.	1.2	219
25	Stilbenoid Dimers:  Dissection of a Paracyclophane Chromophore. Journal of the American Chemical Society, 1998, 120, 9188-9204.	6.6	214
26	Through-Space Charge Transfer and Nonlinear Optical Properties of Substituted Paracyclophane. Journal of the American Chemical Society, 2000, 122, 11956-11962.	6.6	207
27	Direct evidence of quantum transport in photosynthetic light-harvesting complexes. Proceedings of the United States of America, 2011, 108, 20908-20912.	3.3	203
28	Two-Dimensional Raman Spectroscopy of Vibrational Interactions in Liquids. Physical Review Letters, 1997, 79, 2702-2705.	2.9	200
29	Localized Electronic Excitations in Phenylacetylene Dendrimers. Journal of Physical Chemistry B, 1998, 102, 3310-3315.	1.2	198
30	Timeâ€resolved fluorescence and holeâ€burning line shapes of solvated molecules: Longitudinal dielectric relaxation and vibrational dynamics. Journal of Chemical Physics, 1987, 87, 5840-5857.	1.2	191
31	Optical control of molecular dynamics: Molecular cannons, reflectrons, and waveâ€packet focusers. Journal of Chemical Physics, 1993, 99, 6562-6578.	1.2	190
32	Polarons, localization, and excitonic coherence in superradiance of biological antenna complexes. Journal of Chemical Physics, 1997, 107, 3876-3893.	1.2	190
33	Multiple Exciton Coherence Sizes in Photosynthetic Antenna Complexes viewed by Pumpâ^Probe Spectroscopy. Journal of Physical Chemistry B, 1997, 101, 7332-7342.	1.2	188
34	Density-matrix representation of nonadiabatic couplings in time-dependent density functional (TDDFT) theories. Journal of Chemical Physics, 2000, 112, 3572-3579.	1.2	183
35	Temperature-dependent superradiant decay of excitons in small aggregates. Physical Review Letters, 1990, 65, 211-214.	2.9	182
36	Electronic dephasing, vibrational relaxation, and solvent friction in molecular nonlinear optical line shapes. Journal of Chemical Physics, 1988, 89, 5160-5176.	1.2	180

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37	Electrostatic DFT Map for the Complete Vibrational Amide Band of NMA. Journal of Physical Chemistry A, 2005, 109, 9747-9759.	1.1	180
38	Selectivity in coherent transient Raman measurements of vibrational dephasing in liquids. Journal of Chemical Physics, 1985, 83, 2116-2128.	1.2	177
39	Eigenstateâ€free, Green function, calculation of molecular absorption and fluorescence line shapes. Journal of Chemical Physics, 1986, 85, 5908-5923.	1.2	171
40	Multidimensional Attosecond Resonant X-Ray Spectroscopy of Molecules: Lessons from the Optical Regime. Annual Review of Physical Chemistry, 2013, 64, 101-127.	4.8	170
41	Vibrational Sum-Frequency Generation Spectroscopy at the Water/Lipid Interface: Molecular Dynamics Simulation Study. Journal of the American Chemical Society, 2010, 132, 6434-6442.	6.6	167
42	Optical multidimensional coherent spectroscopy. Physics Today, 2013, 66, 44-49.	0.3	167
43	Simulation of the intermolecular vibrational spectra of liquid water and water clusters. Journal of Chemical Physics, 1993, 98, 4413-4421.	1.2	165
44	Photon echoes of polyatomic molecules in condensed phases. Journal of Chemical Physics, 1991, 94, 179-190.	1.2	159
45	Cavity Femtochemistry: Manipulating Nonadiabatic Dynamics at Avoided Crossings. Journal of Physical Chemistry Letters, 2016, 7, 2050-2054.	2.1	158
46	Multidimensional femtosecond correlation spectroscopies of electronic and vibrational excitons. Journal of Chemical Physics, 1999, 110, 5011-5028.	1.2	155
47	Vibrational relaxation in jetâ€cooled alkyl benzenes. II. Fluorescence spectra. Journal of Chemical Physics, 1980, 72, 5049-5061.	1.2	154
48	Coherent Multidimensional Vibrational Spectroscopy of Biomolecules: Concepts, Simulations, and Challenges. Angewandte Chemie - International Edition, 2009, 48, 3750-3781.	7.2	152
49	Multiphoton molecular dissociation in intense laser fields. Journal of Chemical Physics, 1976, 65, 5204-5225.	1.2	149
50	Efficient Fluoride-Selective Fluorescent Host: Experiment and Theoryâ€. Journal of Organic Chemistry, 2004, 69, 943-950.	1.7	146
51	Collisional broadening of spectral line shapes in two-photon and multiphoton processes. Physics Reports, 1982, 93, 1-60.	10.3	145
52	Photon echoes and related fourâ€waveâ€mixing spectroscopies using phaseâ€locked pulses. Journal of Chemical Physics, 1992, 96, 5618-5629.	1.2	145
53	Two-Dimensional Raman Echoes:  Femtosecond View of Molecular Structure and Vibrational Coherence. Accounts of Chemical Research, 1999, 32, 145-154.	7.6	144
54	Collective Solvent Coordinates for the Infrared Spectrum of HOD in D2O Based on an ab Initio Electrostatic Map. Journal of Physical Chemistry A, 2005, 109, 64-82.	1.1	142

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55	Coherent low-frequency motions of hydrogen bonded acetic acid dimers in the liquid phase. Journal of Chemical Physics, 2004, 121, 902-913.	1.2	138
56	Statistical reduction for strongly driven simple quantum systems. Physical Review A, 1978, 17, 1988-1998.	1.0	137
57	Simulation Protocols for Coherent Femtosecond Vibrational Spectra of Peptides. Journal of Physical Chemistry B, 2006, 110, 3362-3374.	1.2	135
58	Theory of vibrational overtone line shapes of polyatomic molecules. Journal of Chemical Physics, 1979, 70, 463.	1.2	132
59	Bacteriochlorophyll and Carotenoid Excitonic Couplings in the LH2 System of Purple Bacteria. Journal of Physical Chemistry B, 2000, 104, 9540-9553.	1.2	127
60	Catching Conical Intersections in the Act: Monitoring Transient Electronic Coherences by Attosecond Stimulated X-Ray Raman Signals. Physical Review Letters, 2015, 115, 193003.	2.9	127
61	Non-markovian theory of molecular relaxation. I. Vibrational relaxation and dephasing in condensed phases. Chemical Physics, 1979, 37, 33-47.	0.9	126
62	Multidimensional femtosecond spectroscopies of molecular aggregates and semiconductor nanostructures: The nonlinear exciton equations. Journal of Chemical Physics, 1998, 109, 9587-9601.	1.2	124
63	Cooperative nonlinear optical response of molecular aggregates: Crossover to bulk behavior. Physical Review Letters, 1991, 66, 1197-1200.	2.9	123
64	Two-Dimensional Real-Space Analysis of Optical Excitations in Acceptor-Substituted Carotenoids. Journal of the American Chemical Society, 1997, 119, 11408-11419.	6.6	123
65	Nonimpact unified theory of four-wave mixing and two-photon processes. Physical Review A, 1983, 28, 3480-3492.	1.0	122
66	The Brownian oscillator model for solvation effects in spontaneous light emission and their relationship to electron transfer. Journal of the American Chemical Society, 1994, 116, 11039-11047.	6.6	121
67	Non-adiabatic dynamics of molecules in optical cavities. Journal of Chemical Physics, 2016, 144, 054309.	1.2	121
68	Molecular theory of solvation and dielectric response in polar fluids. Journal of Chemical Physics, 1987, 87, 1272-1283.	1.2	120
69	Tunneling versus sequential longâ€range electron transfer: Analogy with pump–probe spectroscopy. Journal of Chemical Physics, 1989, 91, 6973-6988.	1.2	120
70	Intermolecular forces, spontaneous emission, and superradiance in a dielectric medium: Polariton-mediated interactions. Physical Review A, 1989, 40, 7065-7080.	1.0	119
71	Real-time path-integral approach to quantum coherence and dephasing in nonadiabatic transitions and nonlinear optical response. Physical Review E, 1993, 47, 118-136.	0.8	119
72	A model for isotope separation via molecular multiphoton photodissociation. Chemical Physics Letters, 1976, 40, 150-156.	1.2	118

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73	Oligophenylenevinylene Phane Dimers:Â Probing the Effect of Contact Site on the Optical Properties of Bichromophoric Pairs. Journal of the American Chemical Society, 2000, 122, 1289-1297.	6.6	116
74	Two-Quantum Many-Body Coherences in Two-Dimensional Fourier-Transform Spectra of Exciton Resonances in Semiconductor Quantum Wells. Physical Review Letters, 2010, 104, 117401.	2.9	115
75	Exciton Hamiltonian for the Bacteriochlorophyll System in the LH2 Antenna Complex of Purple Bacteria. Journal of Physical Chemistry B, 2000, 104, 4519-4528.	1.2	114
76	Exciton Delocalization in the B850 Light-Harvesting Complex:Â Comparison of Different Measures. Journal of Physical Chemistry B, 2001, 105, 5515-5524.	1.2	114
77	Collective coordinates for nuclear spectral densities in energy transfer and femtosecond spectroscopy of molecular aggregates. Journal of Chemical Physics, 1996, 105, 4565-4583.	1.2	113
78	The origin of vibrational mode couplings in various secondary structural motifs of polypeptides. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 506-510.	3.3	113
79	Two-Dimensional Electronic Double-Quantum Coherence Spectroscopy. Accounts of Chemical Research, 2009, 42, 1375-1384.	7.6	113
80	Raman excitation profiles of polyatomic molecules in condensed phases. A stochastic theory. Journal of Chemical Physics, 1986, 85, 462-474.	1.2	112
81	Three-Dimensional Nonlinear Optical Chromophores Based on Through-Space Delocalization. Journal of the American Chemical Society, 2002, 124, 13480-13485.	6.6	112
82	On the semiclassical calculation of molecular absorption and fluorescence spectra. Journal of Chemical Physics, 1982, 77, 173-181.	1.2	111
83	Radiative decay and energy transfer in molecular aggregates: The role of intermolecular dephasing. Physical Review A, 1988, 37, 3835-3846.	1.0	111
84	Classical chaos and fluctuation-dissipation relations for nonlinear response. Physical Review E, 1996, 53, R1-R4.	0.8	109
85	Solvent Reorganization in Long-Range Electron Transfer:Â Density Matrix Approach. Journal of Physical Chemistry A, 1998, 102, 1241-1251.	1.1	108
86	Simulating Coherent Multidimensional Spectroscopy of Nonadiabatic Molecular Processes: From the Infrared to the X-ray Regime. Chemical Reviews, 2017, 117, 12165-12226.	23.0	107
87	Cooperative radiative dynamics in molecular aggregates. Journal of Chemical Physics, 1991, 94, 7534-7544.	1.2	106
88	Lindblad equations for strongly coupled populations and coherences in photosynthetic complexes. Journal of Chemical Physics, 2009, 130, 204512.	1.2	105
89	Nonlinear optical response of conjugated polymers: Electron-hole anharmonic-oscillator picture. Physical Review Letters, 1992, 69, 65-68.	2.9	104
90	Femtosecond photon echoes in molecular aggregates. Journal of Chemical Physics, 1997, 107, 8759-8780.	1.2	101

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91	Roadmap on quantum light spectroscopy. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 072002.	0.6	101
92	Solvation structure and the timeâ€resolved Stokes shift in nonâ€Debye solvents. Journal of Chemical Physics, 1990, 93, 932-946.	1.2	99
93	Signatures of β-Peptide Unfolding in Two-Dimensional Vibrational Echo Spectroscopy: A Simulation Study. Journal of the American Chemical Society, 2001, 123, 3114-3124.	6.6	99
94	Stochastic theory of resonance Raman line shapes of polyatomic molecules in condensed phases. Journal of Chemical Physics, 1985, 82, 5398-5408.	1.2	97
95	Two-Dimensional Double-Quantum Spectra Reveal Collective Resonances in an Atomic Vapor. Physical Review Letters, 2012, 108, 193201.	2.9	97
96	Molecular Structure and Modeling of Water–Air and Ice–Air Interfaces Monitored by Sum-Frequency Generation. Chemical Reviews, 2020, 120, 3633-3667.	23.0	97
97	UV-Light-Induced Vibrational Coherences: The Key to Understand Kasha Rule Violation in <i>trans</i> -Azobenzene. Journal of Physical Chemistry Letters, 2018, 9, 1534-1541.	2.1	96
98	Origin of spectral holes in pump-probe studies of homogeneously broadened lines. Physical Review A, 1984, 29, 1973-1983.	1.0	95
99	Anharmonic oscillator modeling of nonlinear susceptibilities and its application to conjugated polymers. Journal of Chemical Physics, 1994, 100, 2366-2384.	1.2	95
100	Interrogation of Vibrational Structure and Line Broadening of Liquid Water by Raman-Induced Kerr Effect Measurements within the Multimode Brownian Oscillator Model. The Journal of Physical Chemistry, 1996, 100, 10380-10388.	2.9	95
101	Excitonic couplings and electronic coherence in bridged naphthalene dimers. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 13003-13008.	3.3	95
102	Photofragmentation of linear triatomics. Journal of Chemical Physics, 1976, 65, 4035-4048.	1.2	93
103	Multistate quantum Fokker–Planck approach to nonadiabatic wave packet dynamics in pump–probe spectroscopy. Journal of Chemical Physics, 1994, 101, 3049-3061.	1.2	93
104	Superexchange versus sequential long range electron transfer; density matrix pathways in Liouville space. Chemical Physics, 1995, 197, 367-388.	0.9	93
105	Reaction Dynamics of a Photochromic Fluorescing Dithienylethene. Journal of Physical Chemistry A, 2001, 105, 1741-1749.	1.1	93
106	Electronic Coherence and Nonlinear Susceptibilities of Conjugated Polyenes. Science, 1994, 266, 250-254.	6.0	92
107	Lifetimes for resonance fluorescence and near resonance Raman scattering. Journal of Chemical Physics, 1975, 62, 3609.	1.2	91
108	Size Scaling of Third-Order Off-Resonant Polarizabilities. Electronic Coherence in Organic Oligomers. Journal of the American Chemical Society, 2000, 122, 452-459.	6.6	91

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109	Exciton-scaling and optical excitations of self-similar phenylacetylene dendrimers. Journal of Chemical Physics, 1999, 110, 8161-8175.	1.2	90
110	Coherent Multidimensional Optical Probes for Electron Correlations and Exciton Dynamics: From NMR to X-rays. Accounts of Chemical Research, 2009, 42, 553-562.	7.6	90
111	Reaction dynamics of photochromic dithienylethene derivatives. Chemical Physics, 1999, 246, 115-125.	0.9	89
112	Time-resolved x-ray spectroscopies: Nonlinear response functions and Liouville-space pathways. Physical Review A, 2001, 63, .	1.0	88
113	Optically Excited Entangled States in Organic Molecules Illuminate the Dark. Journal of Physical Chemistry Letters, 2013, 4, 2046-2052.	2.1	88
114	Entangled Two-Photon Absorption Spectroscopy. Accounts of Chemical Research, 2018, 51, 2207-2214.	7.6	88
115	Probing intermolecular couplings in liquid water with two-dimensional infrared photon echo spectroscopy. Journal of Chemical Physics, 2008, 128, 191103.	1.2	86
116	Impulsive pump-probe and photon-echo spectroscopies of dye molecules in condensed phases. Physical Review A, 1990, 42, 6920-6923.	1.0	85
117	Design strategies for pulse sequences in multidimensional optical spectroscopies. Journal of Chemical Physics, 2001, 115, 4989-5004.	1.2	85
118	Vibrationalâ^'Exciton Couplings for the Amide I, II, III, and A Modes of Peptides. Journal of Physical Chemistry B, 2007, 111, 11032-11046.	1.2	85
119	Optical Stark Spectroscopy of a Brownian Oscillator in Intense Fields. Journal of the Physical Society of Japan, 1994, 63, 66-77.	0.7	85
120	Superoperator nonequilibrium Green's function theory of many-body systems; applications to charge transfer and transport in open junctions. Physics Reports, 2008, 465, 191-222.	10.3	84
121	Core and valence excitations in resonant X-ray spectroscopy using restricted excitation window time-dependent density functional theory. Journal of Chemical Physics, 2012, 137, 194306.	1.2	83
122	Novel photochemistry of molecular polaritons in optical cavities. Faraday Discussions, 2016, 194, 259-282.	1.6	83
123	Analysis of Absorption Spectra of Zinc Porphyrin, Zinc meso-Tetraphenylporphyrin, and Halogenated Derivatives. Journal of Physical Chemistry A, 2002, 106, 10285-10293.	1.1	81
124	Coherent Multidimensional Optical Spectroscopy. Accounts of Chemical Research, 2009, 42, 1207-1209.	7.6	81
125	Ultrafast Nonlinear Optical Signals Viewed from the Molecule's Perspective. Advances in Atomic, Molecular and Optical Physics, 2010, , 223-263.	2.3	81
126	Collective electronic oscillators for nonlinear optical response of conjugated molecules. Chemical Physics Letters, 1996, 259, 55-61.	1.2	80

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127	Krylov-space algorithms for time-dependent Hartree–Fock and density functional computations. Journal of Chemical Physics, 2000, 113, 36-43.	1.2	79
128	Unified theory of photon echoes: The passage from inhomogeneous to homogeneous line broadening. Chemical Physics Letters, 1985, 114, 426-429.	1.2	78
129	Four-wave mixing and luminescence of confined excitons in molecular aggregates and nanostructures. many-body green function approach. Physics Reports, 1995, 263, 213-309.	10.3	78
130	Suppression of population transport and control of exciton distributions by entangled photons. Nature Communications, 2013, 4, 1782.	5.8	78
131	Molecular fluorescence and near resonance Raman yield as a probe for solvation dynamics. Journal of Chemical Physics, 1987, 86, 6085-6107.	1.2	76
132	Sizeâ€consistent quasiparticle representation of nonlinear optical susceptibilities in manyâ€electron systems. Journal of Chemical Physics, 1996, 104, 444-459.	1.2	76
133	Stochastic Liouville equation simulation of multidimensional vibrational line shapes of trialanine. Journal of Chemical Physics, 2004, 121, 10577-10598.	1.2	76
134	Effective temporal resolution in pump-probe spectroscopy with strongly chirped pulses. Physical Review A, 2010, 82, .	1.0	76
135	Infrared analogs of heteronuclear nuclear magnetic resonance coherence transfer experiments in peptides. Journal of Chemical Physics, 2002, 116, 6803-6816.	1.2	75
136	Nonlinear response of vibrational excitons: Simulating the two-dimensional infrared spectrum of liquid water. Journal of Chemical Physics, 2009, 130, 204110.	1.2	75
137	Exciton-scattering mechanism for enhanced nonlinear response of molecular nanostructures. Physical Review A, 1992, 46, 452-464.	1.0	74
138	Multidimensional femtosecond spectroscopies of vibrational motions in liquids: Semiclassical expansion. Journal of Chemical Physics, 1998, 108, 5812-5825.	1.2	74
139	Superradiance Coherence Sizes in Single-Molecule Spectroscopy of LH2 Antenna Complexes. Journal of Physical Chemistry B, 1999, 103, 3954-3962.	1.2	74
140	Stochastic theory of time-resolved four-wave mixing in interacting media. Physical Review A, 1991, 44, 2124-2129.	1.0	73
141	Coherent Ultrafast Core-Hole Correlation Spectroscopy: X-Ray Analogues of Multidimensional NMR. Physical Review Letters, 2007, 99, 163001.	2.9	73
142	Recursive densityâ€matrixâ€spectralâ€moment algorithm for molecular nonlinear polarizabilities. Journal of Chemical Physics, 1996, 105, 8914-8928.	1.2	72
143	2D-IR Experiments and Simulations of the Coupling between Amide-I and Ionizable Side Chains in Proteins: Application to the Villin Headpiece. Journal of Physical Chemistry B, 2009, 113, 11260-11273.	1.2	72
144	Dielectric friction and the transition from adiabatic to nonadiabatic electron transfer in condensed phases. II. Application to nonâ€Debye solvents. Journal of Chemical Physics, 1988, 88, 4300-4311.	1.2	71

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145	A Quantum Chemical Interpretation of Two-Dimensional Electronic Spectroscopy of Light-Harvesting Complexes. Journal of the American Chemical Society, 2017, 139, 7558-7567.	6.6	71
146	Transient gratings, four-wave mixing and polariton effects in nonlinear optics. Physics Reports, 1991, 205, 1-58.	10.3	69
147	Ultrafast Nonlinear Spectroscopic Techniques in the Gas Phase and Their Density Matrix Representation. Journal of Physical Chemistry A, 2002, 106, 697-718.	1.1	69
148	Stochastic Liouville equations for hydrogen-bonding fluctuations and their signatures in two-dimensional vibrational spectroscopy of water. Journal of Chemical Physics, 2005, 123, 114504.	1.2	69
149	Collisional perturbations of time-resolved photon scattering from molecular levels. Physical Review A, 1975, 12, 947-958.	1.0	68
150	Structure, dynamics, and the electronic absorption of benzene–argon clusters. Journal of Chemical Physics, 1992, 96, 116-135.	1.2	68
151	Simulations of two-dimensional femtosecond infrared photon echoes of glycine dipeptide. Journal of Raman Spectroscopy, 2000, 31, 125-135.	1.2	67
152	Probing valence electronic wave-packet dynamics by all x-ray stimulated Raman spectroscopy: A simulation study. Physical Review A, 2007, 76, .	1.0	67
153	Solvation Effects in Four-Wave Mixing and Spontaneous Raman and Fluorescence Lineshapes of Polyatomic Molecules. Advances in Chemical Physics, 2007, , 165-230.	0.3	66
154	Two-dimensional stimulated resonance Raman spectroscopy of molecules with broadband x-ray pulses. Journal of Chemical Physics, 2012, 136, 174117.	1.2	66
155	Quantum Confined Fano Interference. Physical Review Letters, 1997, 78, 1363-1366.	2.9	65
156	Semiclassical dynamics in Liouville space: Application to molecular electronic spectroscopy. Journal of Chemical Physics, 1988, 88, 5735-5748.	1.2	64
157	Excitons in confined geometries: Size scaling of nonlinear susceptibilities. Journal of Chemical Physics, 1991, 95, 7526-7540.	1.2	64
158	Linear and nonlinear infrared signatures of local α- and 310-helical structures in alanine polypeptides. Journal of Chemical Physics, 2003, 118, 3651-3659.	1.2	64
159	Heat fluctuations and coherences in a quantum heat engine. Physical Review A, 2012, 86, .	1.0	63
160	Chemical Bonding and Size Scaling of Nonlinear Polarizabilities of Conjugated Polymers. Physical Review Letters, 1996, 77, 4656-4659.	2.9	62
161	Simulations of energy funneling and time- and frequency-gated fluorescence in dendrimers. Journal of Chemical Physics, 2001, 114, 2419-2429.	1.2	62
162	Control of Intrachromophore Excitonic Coherence in Electroluminescent Conjugated Dendrimers. Journal of Physical Chemistry B, 2002, 106, 7647-7653.	1.2	62

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163	Electronic density-matrix algorithm for nonadiabatic couplings in molecular dynamics simulations. International Journal of Quantum Chemistry, 2001, 85, 225-238.	1.0	61
164	Pulse shaping and coherent Raman spectroscopy in condensed phases. Journal of Chemical Physics, 1991, 94, 997-1005.	1.2	60
165	Correlated line broadening in multidimensional vibrational spectroscopy. Journal of Chemical Physics, 2002, 117, 11089-11101.	1.2	60
166	Machine Learning Protocol for Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 6026-6031.	2.1	60
167	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. Nature Chemistry, 2021, 13, 343-349.	6.6	59
168	Molecular photodissociation. Journal of Chemical Physics, 1974, 60, 4760-4777.	1.2	58
169	Ultraviolet Spectroscopy of Protein Backbone Transitions in Aqueous Solution: Combined QM and MM Simulations. Journal of Physical Chemistry B, 2010, 114, 8270-8277.	1.2	58
170	Communication: Comment on the effective temporal and spectral resolution of impulsive stimulated Raman signals. Journal of Chemical Physics, 2011, 134, 161101.	1.2	58
171	Monitoring molecular nonadiabatic dynamics with femtosecond X-ray diffraction. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6538-6547.	3.3	58
172	Manipulating nonadiabatic conical intersection dynamics by optical cavities. Chemical Science, 2020, 11, 1290-1298.	3.7	58
173	Nonlinear response functions for birefringence and dichroism measurements in condensed phases. Journal of Chemical Physics, 1993, 98, 5314-5326.	1.2	57
174	Two-dimensional optical spectroscopy of excitons in semiconductor quantum wells: Liouville-space pathway analysis. Physical Review B, 2007, 75, .	1.1	57
175	Multidimensional Infrared Signatures of Intramolecular Hydrogen Bonding in Malonaldehyde. Journal of Physical Chemistry A, 2003, 107, 9113-9131.	1.1	56
176	Nonlinear optical spectroscopy of single, few, and many molecules: Nonequilibrium Green's function QED approach. Physical Review A, 2008, 77, 22110.	1.0	56
177	Double-quantum resonances and exciton-scattering in coherent 2D spectroscopy of photosynthetic complexes. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 8525-8530.	3.3	56
178	Stochastic simulation of chemical exchange in two dimensional infrared spectroscopy. Journal of Chemical Physics, 2006, 125, 014507.	1.2	55
179	Unravelling Coherent Dynamics and Energy Dissipation in Photosynthetic Complexes by 2D Spectroscopy. Biophysical Journal, 2008, 94, 3613-3619.	0.2	55
180	A neural network protocol for electronic excitations of <i>N</i> -methylacetamide. Proceedings of the United States of America, 2019, 116, 11612-11617.	3.3	55

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181	A Machine Learning Protocol for Predicting Protein Infrared Spectra. Journal of the American Chemical Society, 2020, 142, 19071-19077.	6.6	55
182	High-order echoes in vibrational spectroscopy of liquids. Chemical Physics Letters, 1995, 240, 304-314.	1.2	54
183	Extracting single and two-exciton couplings in photosynthetic complexes by coherent two-dimensional electronic spectra. Chemical Physics, 2009, 357, 79-84.	0.9	54
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