Thomas L C Jansen

List of Publications by Year
in descending order

113 papers	5,485 citations	71102 41 h-index	85541 71 g-index
120 all docs	120 docs citations	120 times ranked	4564 citing authors

#	Article	IF	Citations
1	Real-Time Observation of Organic Cation Reorientation in Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 3663-3669.	4.6	322
2	Quantum biology revisited. Science Advances, 2020, 6, eaaz4888.	10.3	266
3	Two-dimensional spectroscopy of a molecular dimer unveils the effects of vibronic coupling on exciton coherences. Nature Chemistry, 2014, 6, 196-201.	13.6	219
4	A transferable electrostatic map for solvation effects on amide I vibrations and its application to linear and two-dimensional spectroscopy. Journal of Chemical Physics, 2006, 124, 044502.	3.0	206
5	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
6	Modeling the amide I bands of small peptides. Journal of Chemical Physics, 2006, 125, 044312.	3.0	202
7	From Atomistic Modeling to Excitation Transfer and Two-Dimensional Spectra of the FMO Light-Harvesting Complex. Journal of Physical Chemistry B, 2011, 115, 8609-8621.	2.6	197
8	Identification and characterization of diverse coherences in the Fennaâ€“Matthewsâ€“Olson complex. Nature Chemistry, 2018, 10, 780-786.	13.6	177
9	Nonadiabatic Effects in the Two-Dimensional Infrared Spectra of Peptides:Â Application to Alanine Dipeptide. Journal of Physical Chemistry B, 2006, 110, 22910-22916.	2.6	174
10	Direct knock-on of desolvated ions governs strict ion selectivity in K+ channels. Nature Chemistry, 2018, 10, 813-820.	13.6	170
11	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.	2.5	142
12	Hydrophobic Solvation: A 2D IR Spectroscopic Inquest. Accounts of Chemical Research, 2009, 42, 1229-1238.	15.6	121
13	Organic Cation Rotation and Immobilization in Pure and Mixed Methylammonium Lead-Halide Perovskites. Journal of the American Chemical Society, 2017, 139, 4068-4074.	13.7	114
14	Two-dimensional infrared spectroscopy and ultrafast anisotropy decay of water. Journal of Chemical Physics, 2010, 132, 224503.	3.0	101
15	Waiting Time Dynamics in Two-Dimensional Infrared Spectroscopy. Accounts of Chemical Research, 2009, 42, 1405-1411.	15.6	98
16	Melting of a Î²-Hairpin Peptide Using Isotope-Edited 2D IR Spectroscopy and Simulations. Journal of Physical Chemistry B, 2010, 114, 10913-10924.	2.6	97
17	The third- and fifth-order nonlinear Raman response of liquid CS2 calculated using a finite field nonequilibrium molecular dynamics method. Journal of Chemical Physics, 2000, 113, 307-311.	3.0	93
18	Spatially-resolved fluorescence-detected two-dimensional electronic spectroscopy probes varying excitonic structure in photosynthetic bacteria. Nature Communications, 2018, 9, 4219.	12.8	86

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19	Dynamics of Water Confined in Reversed Micelles: Multidimensional Vibrational Spectroscopy Study. Journal of Physical Chemistry B, 2013, 117, 15545-15558.	2.6	82
20	Interaction induced effects in the nonlinear Raman response of liquid CS2: A finite field nonequilibrium molecular dynamics approach. Journal of Chemical Physics, 2001, 114, 10910-10921.	3.0	80
21	Stochastic Liouville equation simulation of multidimensional vibrational line shapes of trialanine. Journal of Chemical Physics, 2004, 121, 10577-10598.	3.0	76
22	An Efficient N³-Scaling Propagation Scheme for Simulating Two-Dimensional Infrared and Visible Spectra. Journal of Chemical Theory and Computation, 2012, 8, 1706-1713.	5.3	71
23	Stochastic Liouville equations for hydrogen-bonding fluctuations and their signatures in two-dimensional vibrational spectroscopy of water. Journal of Chemical Physics, 2005, 123, 114504.	3.0	69
24	Vibrational Beatings Conceal Evidence of Electronic Coherence in the FMO Light-Harvesting Complex. Journal of Physical Chemistry B, 2014, 118, 12865-12872.	2.6	68
25	Rotational Cation Dynamics in Metal Halide Perovskites: Effect on Phonons and Material Properties. Journal of Physical Chemistry Letters, 2018, 9, 5987-5997.	4.6	68
26	Simulation of vibrational energy transfer in two-dimensional infrared spectroscopy of amide I and amide II modes in solution. Journal of Chemical Physics, 2008, 129, 055101.	3.0	59
27	Atomistic Modeling of Two-Dimensional Electronic Spectra and Excited-State Dynamics for a Light Harvesting 2 Complex. Journal of Physical Chemistry B, 2015, 119, 1302-1313.	2.6	59
28	Solvent and conformation dependence of amide I vibrations in peptides and proteins containing proline. Journal of Chemical Physics, 2011, 135, 234507.	3.0	58
29	Surface hopping modeling of two-dimensional spectra. Journal of Chemical Physics, 2013, 138, 164106.	3.0	58
30	Two-Dimensional Infrared Population Transfer Spectroscopy for Enhancing Structural Markers of Proteins. Biophysical Journal, 2008, 94, 1818-1825.	0.5	57
31	Calculating Two-Dimensional Spectra with the Mixed Quantum-Classical Ehrenfest Method. Journal of Physical Chemistry A, 2013, 117, 5970-5980.	2.5	54
32	Exciton mobility control through<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>sub</mml:mtext><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">Ã…</mml:mi></mml:math>packing modifications in molecular crystals. Physical Review B, 2015, 91, .	3.2	51
33	Dissimilar Dynamics of Coupled Water Vibrations. Journal of Physical Chemistry A, 2009, 113, 6260-6265.	2.5	50
34	Identifying Residual Structure in Intrinsically Disordered Systems: A 2D IR Spectroscopic Study of the GVGXPGVG Peptide. Journal of the American Chemical Society, 2012, 134, 5032-5035.	13.7	48
35	Mapping the Evolution of Spatial Exciton Coherence through Time-Resolved Fluorescence. Journal of Physical Chemistry Letters, 2014, 5, 1505-1510.	4.6	47
36	Ultrafast anisotropy dynamics of water molecules dissolved in acetonitrile. Journal of Chemical Physics, 2007, 127, 084507.	3.0	45

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37	Structural classification of the amide I sites of a Î²-hairpin with isotope label 2DIR spectroscopy. Physical Chemistry Chemical Physics, 2010, 12, 9347.	2.8	45
38	On the nature of OH-stretching vibrations in hydrogen-bonded chains: Pump frequency dependent vibrational lifetime. Physical Chemistry Chemical Physics, 2011, 13, 4641.	2.8	45
39	Localization and coherent dynamics of excitons in the two-dimensional optical spectrum of molecular J-aggregates. Journal of Chemical Physics, 2008, 128, 164511.	3.0	44
40	Analysis of 2D CS Spectra for Systems with Non-Gaussian Dynamics. Journal of Physical Chemistry B, 2011, 115, 5431-5440.	2.6	44
41	Interplay between structural hierarchy and exciton diffusion in artificial light harvesting. Nature Communications, 2019, 10, 4615.	12.8	44
42	The Primary Photochemistry of Vision Occurs at the Molecular Speed Limit. Journal of Physical Chemistry B, 2017, 121, 4040-4047.	2.6	42
43	Theory of coherent two-dimensional vibrational spectroscopy. Journal of Chemical Physics, 2019, 150, 100901.	3.0	40
44	Interplay between Hydrogen Bonding and Vibrational Coupling in Liquid N-Methylacetamide. Journal of Physical Chemistry Letters, 2017, 8, 2438-2444.	4.6	38
45	Excitonâ€“Exciton Annihilation Is Coherently Suppressed in H-Aggregates, but Not in J-Aggregates. Journal of Physical Chemistry Letters, 2017, 8, 6113-6117.	4.6	38
46	Structural and Spectroscopic Properties of Assemblies of Self-Replicating Peptide Macrocycles. ACS Nano, 2017, 11, 7858-7868.	14.6	36
47	Application of two-dimensional infrared spectroscopy to benchmark models for the amide I band of proteins. Journal of Chemical Physics, 2015, 142, 212437.	3.0	34
48	Steering Self-Assembly of Amphiphilic Molecular Nanostructures via Halogen Exchange. Journal of Physical Chemistry Letters, 2017, 8, 2895-2901.	4.6	34
49	Close collisions in the two-dimensional Raman response of liquid carbon disulfide. Physical Review B, 2003, 67, .	3.2	33
50	Hydrogen bond dynamics in bulk alcohols. Journal of Chemical Physics, 2015, 142, 212450.	3.0	32
51	Assessing Spectral Simulation Protocols for the Amide I Band of Proteins. Journal of Chemical Theory and Computation, 2016, 12, 3982-3992.	5.3	32
52	Tunable Ferroelectricity in Ruddlesdenâ€“Popper Halide Perovskites. ACS Applied Materials & Interfaces, 2019, 11, 13523-13532.	8.0	32
53	Linear Absorption and Two-Dimensional Infrared Spectra of N-Methylacetamide in Chloroform Revisited: Polarizability and Multipole Effects. Journal of Physical Chemistry B, 2014, 118, 8162-8169.	2.6	31
54	Modeling the Vibrational Dynamics and Nonlinear Infrared Spectra of Coupled Amide I and II Modes in Peptides. Journal of Physical Chemistry B, 2011, 115, 5392-5401.	2.6	27

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55	Computational spectroscopy of complex systems. Journal of Chemical Physics, 2021, 155, 170901.	3.0	27
56	Collision effects in the nonlinear Raman response of liquid carbon disulfide. Journal of Chemical Physics, 2002, 116, 3277-3285.	3.0	26
57	Two-dimensional infrared spectroscopy of neat ice I_h. Physical Chemistry Chemical Physics, 2016, 18, 3772-3779.	2.8	26
58	Simulating Fluorescence-Detected Two-Dimensional Electronic Spectroscopy of Multichromophoric Systems. Journal of Physical Chemistry B, 2019, 123, 394-406.	2.6	26
59	Fifth-Order Raman Spectroscopy of Liquid Benzene:Â Experiment and Theoryâ€. Journal of Physical Chemistry B, 2006, 110, 19867-19876.	2.6	24
60	Calculation of two-dimensional infrared spectra of ultrafast chemical exchange with numerical Langevin simulations. Journal of Chemical Physics, 2007, 127, 234502.	3.0	24
61	Hydrophobic Collapse in N-Methylacetamideâ€“Water Mixtures. Journal of Physical Chemistry A, 2018, 122, 2468-2478.	2.5	23
62	Soft Xâ€ray Spectroscopy as a Probe for Gasâ€Phase Protein Structure: Electron Impact Ionization from Within. Chemistry - A European Journal, 2018, 24, 7631-7636.	3.3	23
63	Vibrational Spectra of a Mechanosensitive Channel. Journal of Physical Chemistry Letters, 2013, 4, 448-452.	4.6	22
64	Vibrational relaxation in simulated two-dimensional infrared spectra of two amide modes in solution. Journal of Chemical Physics, 2007, 127, 194505.	3.0	21
65	Motional narrowing in the time-averaging approximation for simulating two-dimensional nonlinear infrared spectra. Journal of Chemical Physics, 2008, 128, 214501.	3.0	21
66	Probing the Interstate Coupling near a Conical Intersection by Optical Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 3328-3334.	4.6	20
67	Spectral and Structural Variations of Biomimetic Light-Harvesting Nanotubes. Journal of Physical Chemistry Letters, 2019, 10, 2715-2724.	4.6	20
68	Semiclassical mode-coupling factorizations of coherent nonlinear optical response. Journal of Chemical Physics, 2003, 119, 7979-7987.	3.0	19
69	Laser-Limited Signatures of Quantum Coherence. Journal of Physical Chemistry A, 2016, 120, 3042-3048.	2.5	19
70	Time correlation function and finite field approaches to the calculation of the fifth order Raman response in liquid xenon. Journal of Chemical Physics, 2006, 125, 234501.	3.0	18
71	Structural Variations in Chlorosomes from Wild-Type and a bchQR Mutant of Chlorobaculum tepidum Revealed by Single-Molecule Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 6712-6723.	2.6	18
72	Multiscale modeling of molecular structure and optical properties of complex supramolecular aggregates. Chemical Science, 2020, 11, 11514-11524.	7.4	18

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73	Simulation of Two-Dimensional Sum-Frequency Generation Response Functions: Application to Amide I in Proteins. Journal of Physical Chemistry B, 2013, 117, 6937-6945.	2.6	16
74	OH-Stretching in Synthetic Hydrogen-Bonded Chains. Journal of Physical Chemistry B, 2014, 118, 6256-6264.	2.6	16
75	Proton transport in biological systems can be probed by two-dimensional infrared spectroscopy. Journal of Chemical Physics, 2011, 134, 044502.	3.0	14
76	2D IR spectroscopy of high-pressure phases of ice. Journal of Chemical Physics, 2017, 147, 144501.	3.0	14
77	The origin of absorptive features in the two-dimensional electronic spectra of rhodopsin. Physical Chemistry Chemical Physics, 2018, 20, 12746-12754.	2.8	14
78	Comparison of methods to study excitation energy transfer in molecular multichromophoric systems. Chemical Physics, 2020, 529, 110478.	1.9	14
79	Exciton localization in tubular molecular aggregates: Size effects and optical response. Journal of Chemical Physics, 2020, 152, 194302.	3.0	14
80	Molecular versus Excitonic Disorder in Individual Artificial Light-Harvesting Systems. Journal of the American Chemical Society, 2020, 142, 18073-18085.	13.7	13
81	Observation of Ultrafast Coherence Transfer and Degenerate States with Polarization-Controlled Two-Dimensional Electronic Spectroscopy. Journal of Physical Chemistry B, 2020, 124, 9420-9427.	2.6	13
82	Temperature-Induced Collapse of Elastin-like Peptides Studied by 2DIR Spectroscopy. Journal of Physical Chemistry B, 2018, 122, 8243-8254.	2.6	12
83	Spectral line shapes in linear absorption and two-dimensional spectroscopy with skewed frequency distributions. Journal of Chemical Physics, 2017, 146, 234201.	3.0	11
84	Many-body effects in the stimulated Raman response of binary mixtures: A comparison between theory and experiment. Journal of Chemical Physics, 2002, 116, 9383-9391.	3.0	10
85	Two-Dimensional Spectroscopy of Extended Molecular Systems: Applications to Energy Transport and Relaxation in an Î±-Helix. Journal of Physical Chemistry A, 2010, 114, 7315-7320.	2.5	10
86	Charge Recombination Suppressed by Destructive Quantum Interference in Heterojunction Materials. Journal of Physical Chemistry Letters, 2016, 7, 198-203.	4.6	10
87	Excited state dynamics and exciton diffusion in triphenylamine/dicyanovinyl pushâ€“pull small molecule for organic optoelectronics. Scientific Reports, 2020, 10, 21198.	3.3	10
88	Experimental and Theoretical Investigation of the UV Spectrum and Kinetics of the Aminomethyl Radical, CH2NH2.. Acta Chemica Scandinavica, 1999, 53, 1054-1058.	0.7	10
89	Hydrogen bond and lifetime dynamics in diluted alcohols. Physical Chemistry Chemical Physics, 2017, 19, 27960-27967.	2.8	9
90	Simple Quantum Dynamics with Thermalization. Journal of Physical Chemistry A, 2018, 122, 172-183.	2.5	9

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91	Proton Transport in a Membrane Protein Channel: Two-Dimensional Infrared Spectrum Modeling. Journal of Physical Chemistry B, 2012, 116, 6336-6345.	2.6	8
92	Suppressing sampling noise in linear and two-dimensional spectral simulations. Journal of Chemical Physics, 2015, 142, 054201.	3.0	8
93	Lessons from combined experimental and theoretical examination of the FTIR and 2D-IR spectroelectrochemistry of the amide I region of cytochrome c. Journal of Chemical Physics, 2021, 154, 124201.	3.0	8
94	AIM: A Mapping Program for Infrared Spectroscopy of Proteins. Journal of Chemical Theory and Computation, 2022, 18, 3089-3098.	5.3	8
95	Proton transport in a binary biomimetic solution revealed by molecular dynamics simulation. Journal of Chemical Physics, 2011, 135, 114502.	3.0	7
96	Ultrafast Excitation Energy Transfer Dynamics in the LHCIIâ€“CP29â€“CP24 Subdomain of Plant Photosystem II. Journal of Physical Chemistry Letters, 2022, 13, 4263-4271.	4.6	7
97	On the evaluation of spin-orbit coupling matrix elements in a spin-adapted basis. International Journal of Quantum Chemistry, 1999, 73, 23-27.	2.0	6
98	Liquid xenon as an ideal probe for many-body effects in impulsive Raman scattering. Journal of Chemical Physics, 2002, 117, 1181-1187.	3.0	6
99	Quantum-Classical Simulation of Molecular Motors Driven Only by Light. Journal of Physical Chemistry Letters, 2021, 12, 5512-5518.	4.6	5
100	Distinguishing islet amyloid polypeptide fibril structures with infrared isotope-label spectroscopy. Journal of Chemical Physics, 2022, 156, 055101.	3.0	5
101	Unraveling intra-aggregate structural disorder using single-molecule spectroscopy. Journal of Chemical Physics, 2020, 153, 134304.	3.0	4
102	An Exciton Dynamics Model of Bryopsis corticulans Light-Harvesting Complex II. Journal of Physical Chemistry B, 2021, 125, 1134-1143.	2.6	4
103	Scaling relations of exciton diffusion in linear aggregates with static and dynamic disorder. Journal of Chemical Physics, 2021, 155, 134305.	3.0	4
104	Signatures of Chemical Exchange in 2D Vibrational Spectroscopy; Simulations Based on the Stochastic Liouville Equations. Springer Series in Chemical Physics, 2007, , 401-403.	0.2	3
105	Unraveling Molecular Packing in Two-Dimensional Excitonic Systems. CheM, 2019, 5, 3010-3012.	11.7	2
106	Probing size variations of molecular aggregates inside chlorosomes using single-object spectroscopy. Journal of Chemical Physics, 2021, 155, 124310.	3.0	2
107	Optical Signatures of the Coupling between Excitons and Charge Transfer States in Linear Molecular Aggregates. Journal of Chemical Physics, 0, , .	3.0	1
108	The Effect of Induced Multipoles on the Fifth-order Raman Response. Bulletin of the Korean Chemical Society, 2003, 24, 1102-1106.	1.9	0

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109	Fifth-order Raman spectroscopy: Liquid benzene. , 2006, , .		0
110	Fifth-order Raman spectroscopy: Liquid benzene. Springer Series in Chemical Physics, 2007, , 297-299.	0.2	0
111	Heterogeneous Dynamics of Coupled Vibrations. Springer Series in Chemical Physics, 2009, , 472-474.	0.2	0
112	Hydrogen Bond Dynamics in Alcohols Studied by 2D IR Spectroscopy. , 2014, , .		0
113	Hydrogen Bond Dynamics in Alcohols Studied by 2D IR Spectroscopy. Springer Proceedings in Physics, 2015, , 466-470.	0.2	0