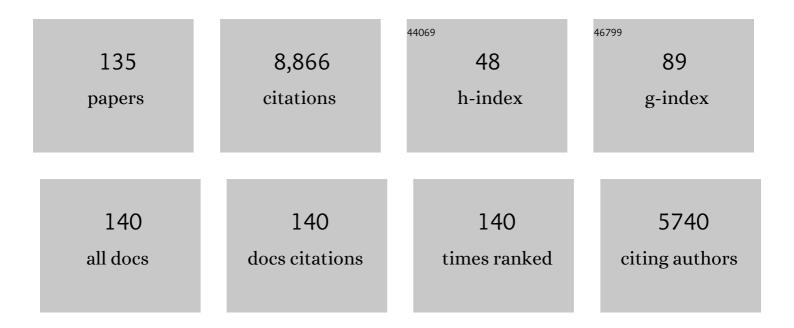
Gerhard Stock

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Semiclassical Description of Nonadiabatic Quantum Dynamics. Physical Review Letters, 1997, 78, 578-581.	7.8	456
2	Energy landscape of a small peptide revealed by dihedral angle principal component analysis. Proteins: Structure, Function and Bioinformatics, 2004, 58, 45-52.	2.6	363
3	Monomer adds to preformed structured oligomers of Abeta-peptides by a two-stage dock-lock mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 111-116.	7.1	344
4	Structure and Dynamics of the Homologous Series of Alanine Peptides:Â A Joint Molecular Dynamics/NMR Study. Journal of the American Chemical Society, 2007, 129, 1179-1189.	13.7	304
5	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
6	Dihedral angle principal component analysis of molecular dynamics simulations. Journal of Chemical Physics, 2007, 126, 244111.	3.0	279
7	Surface-hopping modeling of photoinduced relaxation dynamics on coupled potential-energy surfaces. Journal of Chemical Physics, 1997, 107, 6230-6245.	3.0	239
8	Peptide conformational heterogeneity revealed from nonlinear vibrational spectroscopy and molecular-dynamics simulations. Journal of Chemical Physics, 2002, 117, 6833-6840.	3.0	219
9	Mapping approach to the semiclassical description of nonadiabatic quantum dynamics. Physical Review A, 1999, 59, 64-79.	2.5	213
10	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
11	Conformational Dynamics of Trialanine in Water. 2. Comparison of AMBER, CHARMM, GROMOS, and OPLS Force Fields to NMR and Infrared Experiments. Journal of Physical Chemistry B, 2003, 107, 5064-5073.	2.6	199
12	Nonperturbative approach to femtosecond spectroscopy: General theory and application to multidimensional nonadiabatic photoisomerization processes. Journal of Chemical Physics, 1995, 103, 3998-4011.	3.0	197
13	A PELDOR-Based Nanometer Distance Ruler for Oligonucleotides. Journal of the American Chemical Society, 2004, 126, 5722-5729.	13.7	193
14	Energy transport in peptide helices. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 12749-12754.	7.1	179
15	Construction of the free energy landscape of biomolecules via dihedral angle principal component analysis. Journal of Chemical Physics, 2008, 128, 245102.	3.0	170
16	Semiclassical description of nonadiabatic quantum dynamics: Application to the S1–S2 conical intersection in pyrazine. Journal of Chemical Physics, 2000, 112, 10282-10292.	3.0	155
17	Quantum-Mechanical Modeling of the Femtosecond Isomerization in Rhodopsin. Journal of Physical Chemistry B, 2000, 104, 1146-1149.	2.6	151
18	Principal component analysis of molecular dynamics: On the use of Cartesian vs. internal coordinates. Journal of Chemical Physics, 2014, 141, 014111.	3.0	149

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19	Base-specific spin-labeling of RNA for structure determination. Nucleic Acids Research, 2007, 35, 3128-3143.	14.5	146
20	Ab initio-based exciton model of amide I vibrations in peptides: Definition, conformational dependence, and transferability. Journal of Chemical Physics, 2005, 122, 224904.	3.0	127
21	Free energy landscape and folding mechanism of a β-hairpin in explicit water: A replica exchange molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 61, 795-808.	2.6	125
22	Flow of zero-point energy and exploration of phase space in classical simulations of quantum relaxation dynamics. Journal of Chemical Physics, 1999, 111, 65-76.	3.0	117
23	Flow of zero-point energy and exploration of phase space in classical simulations of quantum relaxation dynamics. II. Application to nonadiabatic processes. Journal of Chemical Physics, 1999, 111, 77-88.	3.0	107
24	Perspective: Identification of collective variables and metastable states of protein dynamics. Journal of Chemical Physics, 2018, 149, 150901.	3.0	105
25	A semiclassical selfâ€consistentâ€field approach to dissipative dynamics: The spin–boson problem. Journal of Chemical Physics, 1995, 103, 1561-1573.	3.0	100
26	Energy Transport in Peptide Helices: A Comparison between High- and Low-Energy Excitations. Journal of Physical Chemistry B, 2008, 112, 9091-9099.	2.6	92
27	Detection of ultrafast molecular-excited-state dynamics with time- and frequency-resolved pump-probe spectroscopy. Physical Review A, 1992, 45, 3032-3040.	2.5	90
28	How Complex Is the Dynamics of Peptide Folding?. Physical Review Letters, 2007, 98, 028102.	7.8	85
29	Conformational Dynamics of Trialanine in Water:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2002, 106, 5294-5301.	2.6	83
30	Resonance Raman spectroscopy of theS1andS2states of pyrazine: Experiment and first principles calculation of spectra. Journal of Chemical Physics, 1995, 103, 6851-6860.	3.0	81
31	Nonequilibrium molecular-dynamics study of the vibrational energy relaxation of peptides in water. Journal of Chemical Physics, 2003, 119, 11350-11358.	3.0	80
32	Quantum-classical Liouville description of multidimensional nonadiabatic molecular dynamics. Journal of Chemical Physics, 2001, 114, 2001-2012.	3.0	79
33	Identifying Metastable States of Folding Proteins. Journal of Chemical Theory and Computation, 2012, 8, 3810-3819.	5.3	74
34	Contact- and distance-based principal component analysis of protein dynamics. Journal of Chemical Physics, 2015, 143, 244114.	3.0	74
35	Molecular dynamics simulation study of the binding of purine bases to the aptamer domain of the guanine sensing riboswitch. Nucleic Acids Research, 2009, 37, 4774-4786.	14.5	72
36	Inferring Transition Rates of Networks from Populations in Continuous-Time Markov Processes. Journal of Chemical Theory and Computation, 2015, 11, 5464-5472.	5.3	69

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37	Robust Density-Based Clustering To Identify Metastable Conformational States of Proteins. Journal of Chemical Theory and Computation, 2016, 12, 2426-2435.	5.3	68
38	Consistent treatment of quantum-mechanical and classical degrees of freedom in mixed quantum-classical simulations. Journal of Chemical Physics, 1998, 108, 7516-7526.	3.0	67
39	Nonequilibrium molecular dynamics simulation of the energy transport through a peptide helix. Journal of Chemical Physics, 2010, 132, 025102.	3.0	66
40	Classical Simulation of Quantum Energy Flow in Biomolecules. Physical Review Letters, 2009, 102, 118301.	7.8	65
41	Machine Learning of Biomolecular Reaction Coordinates. Journal of Physical Chemistry Letters, 2018, 9, 2144-2150.	4.6	65
42	Time-resolved observation of protein allosteric communication. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6804-E6811.	7.1	63
43	A semiclassical selfâ€consistentâ€field approach to dissipative dynamics. II. Internal conversion processes. Journal of Chemical Physics, 1995, 103, 2888-2902.	3.0	60
44	Nonequilibrium molecular dynamics simulation of a photoswitchable peptide. Chemical Physics, 2006, 323, 36-44.	1.9	60
45	Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach. Chemical Physics, 1997, 217, 275-287.	1.9	56
46	NMR and MD studies of the temperature-dependent dynamics of RNA YNMG-tetraloops. Nucleic Acids Research, 2008, 36, 1928-1940.	14.5	56
47	Structural Flexibility of a Helical Peptide Regulates Vibrational Energy Transport Properties. Journal of Physical Chemistry B, 2008, 112, 15487-15492.	2.6	53
48	Free-Energy Landscape of RNA Hairpins Constructed via Dihedral Angle Principal Component Analysis. Journal of Physical Chemistry B, 2009, 113, 16660-16668.	2.6	53
49	Multisecond ligand dissociation dynamics from atomistic simulations. Nature Communications, 2020, 11, 2918.	12.8	52
50	Femtosecond secondary emission arising from the nonadiabatic photoisomerization in rhodopsin. Chemical Physics, 2000, 259, 297-312.	1.9	50
51	Principal component analysis on a torus: Theory and application to protein dynamics. Journal of Chemical Physics, 2017, 147, 244101.	3.0	50
52	Photoinduced Conformational Dynamics of a Photoswitchable Peptide: A Nonequilibrium Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 91, 1224-1234.	0.5	49
53	Maximum Caliber: A variational approach applied to two-state dynamics. Journal of Chemical Physics, 2008, 128, 194102.	3.0	49
54	Multidimensional Langevin modeling of biomolecular dynamics. Journal of Chemical Physics, 2009, 130, 034106.	3.0	48

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55	Vibrational energy flow in the villin headpiece subdomain: Master equation simulations. Journal of Chemical Physics, 2015, 142, 075101.	3.0	48
56	Scaling Rules for Vibrational Energy Transport in Globular Proteins. Journal of Physical Chemistry Letters, 2016, 7, 25-30.	4.6	48
57	Metadynamics Enhanced Markov Modeling of Protein Dynamics. Journal of Physical Chemistry B, 2018, 122, 5508-5514.	2.6	48
58	A non-equilibrium approach to allosteric communication. Philosophical Transactions of the Royal Society B: Biological Sciences, 2018, 373, 20170187.	4.0	48
59	Molecular Dynamics Simulation of the Structure, Dynamics, and Thermostability of the RNA Hairpins uCACGg and cUUCGg. Journal of Physical Chemistry B, 2008, 112, 134-142.	2.6	47
60	Mechanism of a photochemical funnel: a dissipative wave-packet dynamics study. Chemical Physics Letters, 2003, 379, 351-358.	2.6	45
61	Structure and energy landscape of a photoswitchable peptide: A replica exchange molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 60, 485-494.	2.6	45
62	Real-time observation of ligand-induced allosteric transitions in a PDZ domain. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26031-26039.	7.1	45
63	SYNTHESIS OF SPIN-LABELED RNAS FOR LONG RANGE DISTANCE MEASUREMENTS BY PELDOR. Nucleosides, Nucleotides and Nucleic Acids, 2005, 24, 771-775.	1.1	44
64	Molecular dynamics simulation of cooling: Heat transfer from a photoexcited peptide to the solvent. Journal of Chemical Physics, 2009, 131, 184503.	3.0	41
65	Targeted Molecular Dynamics Calculations of Free Energy Profiles Using a Nonequilibrium Friction Correction. Journal of Chemical Theory and Computation, 2018, 14, 6175-6182.	5.3	41
66	Construction of the Free Energy Landscape of Peptide Aggregation from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 1471-1479.	5.3	40
67	Ultrafastcis-transphotoswitching: A model study. Journal of Chemical Physics, 2002, 116, 1085-1091.	3.0	39
68	What NMR Relaxation Can Tell Us about the Internal Motion of an RNA Hairpin:  A Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2006, 2, 1228-1236.	5.3	39
69	Hierarchical Folding Free Energy Landscape of HP35 Revealed by Most Probable Path Clustering. Journal of Physical Chemistry B, 2014, 118, 7750-7760.	2.6	39
70	Vibrational Conical Intersections as a Mechanism of Ultrafast Vibrational Relaxation. Physical Review Letters, 2012, 109, 173201.	7.8	38
71	Energy Flow and Long-Range Correlations in Guanine-Binding Riboswitch: A Nonequilibrium Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 9340-9347.	2.6	36
72	Structure and Dynamics of an RNA Tetraloop: A Joint Molecular Dynamics and NMR Study. Structure, 2005, 13, 1255-1267.	3.3	35

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73	Conformational Dynamics of RNA-Peptide Binding: A Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 90, 391-399.	0.5	35
74	Identification and Validation of Reaction Coordinates Describing Protein Functional Motion: Hierarchical Dynamics of T4 Lysozyme. Journal of Chemical Theory and Computation, 2017, 13, 5076-5088.	5.3	35
75	Ab initio based building block model of amide I vibrations in peptides. Chemical Physics Letters, 2007, 437, 272-276.	2.6	33
76	Photocontrolling Protein–Peptide Interactions: From Minimal Perturbation to Complete Unbinding. Journal of the American Chemical Society, 2019, 141, 10702-10710.	13.7	33
77	Principal component analysis of nonequilibrium molecular dynamics simulations. Journal of Chemical Physics, 2019, 150, 204110.	3.0	31
78	Classical description of nonadiabatic photoisomerization processes and their realâ€ŧime detection via femtosecond spectroscopy. Journal of Chemical Physics, 1995, 103, 10015-10029.	3.0	30
79	Dynamic treatment of vibrational energy relaxation in a heterogeneous and fluctuating environment. Journal of Chemical Physics, 2008, 129, 134110.	3.0	30
80	Hierarchical Biomolecular Dynamics: Picosecond Hydrogen Bonding Regulates Microsecond Conformational Transitions. Journal of Chemical Theory and Computation, 2015, 11, 1330-1336.	5.3	30
81	Modeling of decoherence and dissipation in nonadiabatic photoreactions by an effective-scaling nonsecular Redfield algorithm. Chemical Physics, 2005, 310, 33-41.	1.9	29
82	Through bonds or contacts? Mapping protein vibrational energy transfer using non-canonical amino acids. Nature Communications, 2021, 12, 3284.	12.8	28
83	Efficient calculation of femtosecond time-resolved photoelectron spectra: method and application to the ionization of pyrazine. Physical Chemistry Chemical Physics, 2001, 3, 2331-2336.	2.8	27
84	Long-Range Conformational Transition of a Photoswitchable Allosteric Protein: Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 13468-13476.	2.6	26
85	Dynamical coring of Markov state models. Journal of Chemical Physics, 2019, 150, 094111.	3.0	26
86	Nonadiabatic vibrational dynamics and spectroscopy of peptides: A quantum-classical description. Chemical Physics, 2008, 347, 208-217.	1.9	24
87	Hidden Complexity of Protein Free-Energy Landscapes Revealed by Principal Component Analysis by Parts. Journal of Physical Chemistry Letters, 2010, 1, 2769-2773.	4.6	24
88	Classical formulation of the spectroscopy of nonadiabatic excitedâ€state dynamics. Journal of Chemical Physics, 1993, 99, 1545-1555.	3.0	23
89	Long-Range Conformational Response of a PDZ Domain to Ligand Binding and Release: A Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2016, 12, 870-878.	5.3	23
90	Quantum and classical vibrational relaxation dynamics of <i>N</i> â€methylacetamide on ab initio potential energy surfaces. International Journal of Quantum Chemistry, 2009, 109, 2047-2057.	2.0	22

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91	Vibrational conical intersections in the water dimer. Molecular Physics, 2013, 111, 2046-2056.	1.7	22
92	A Numerical Procedure to Evaluate Memory Effects in Nonâ€Equilibrium Coarseâ€Grained Models. Advanced Theory and Simulations, 2021, 4, 2000197.	2.8	22
93	Hierarchical dynamics in allostery following ATP hydrolysis monitored by single molecule FRET measurements and MD simulations. Chemical Science, 2021, 12, 3350-3359.	7.4	22
94	Classical description of ultrafast internal conversion processes. The benzene cation. Chemical Physics Letters, 1994, 224, 131-138.	2.6	21
95	Approximate calculation of femtosecond pump–probe spectra monitoring nonadiabatic excited-state dynamics. Journal of Chemical Physics, 2000, 112, 4910-4922.	3.0	21
96	A classical model for time- and frequency-resolved spectroscopy of nonadiabatic excited-state dynamics. Chemical Physics Letters, 1992, 197, 396-404.	2.6	20
97	Multidimensional Langevin Modeling of Nonoverdamped Dynamics. Physical Review Letters, 2015, 115, 050602.	7.8	20
98	Nonadiabatic vibrational dynamics in the HCO2â~'â‹H2O complex. Journal of Chemical Physics, 2015, 143, 134308.	3.0	20
99	Model studies on femtosecond spectroscopy of multidimensional photoisomerization and internal-conversion dynamics. A nonperturbative approach. Chemical Physics Letters, 1994, 228, 665-671.	2.6	19
100	Quasiperiodic orbit analysis of nonadiabaticcis–transphotoisomerization dynamics. Journal of Chemical Physics, 2003, 119, 4204-4215.	3.0	18
101	Transient Spectral Features of a cisâ~'trans Photoreaction in the Condensed Phase:  A Model Study. Journal of Physical Chemistry A, 2004, 108, 6464-6473.	2.5	18
102	2D-IR Spectroscopy of an AHA Labeled Photoswitchable PDZ2 Domain. Journal of Physical Chemistry A, 2017, 121, 9435-9445.	2.5	18
103	Azidohomoalanine: A Minimally Invasive, Versatile, and Sensitive Infrared Label in Proteins To Study Ligand Binding. Journal of Physical Chemistry B, 2018, 122, 10118-10125.	2.6	18
104	Efficient calculation of time- and frequency-resolved spectra: a mixed non-perturbative/perturbative approach. Chemical Physics Letters, 1998, 296, 137-145.	2.6	16
105	Model study on the real-time detection of ultrafast nonadiabatic dynamics associated with the Wulf-Chappuis bands of ozone. Chemical Physics Letters, 1992, 200, 163-172.	2.6	15
106	Energy Transport Pathways in Proteins: A Non-equilibrium Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2019, 15, 5750-5757.	5.3	15
107	Master equation model to predict energy transport pathways in proteins. Journal of Chemical Physics, 2020, 152, 045103.	3.0	14
108	Real Time Observation of Ultrafast Peptide Conformational Dynamics: Molecular Dynamics Simulation vs Infrared Experiment. Journal of Physical Chemistry B, 2011, 115, 13084-13092.	2.6	13

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109	MELD-Path Efficiently Computes Conformational Transitions, Including Multiple and Diverse Paths. Journal of Chemical Theory and Computation, 2018, 14, 2109-2116.	5.3	13
110	MSMPathfinder: Identification of Pathways in Markov State Models. Journal of Chemical Theory and Computation, 2020, 16, 7874-7882.	5.3	13
111	Periodic Orbit Description of Nonadiabatic Quantum Dynamics. Physical Review Letters, 2001, 87, 140404.	7.8	12
112	Quasiclassical and semiclassical wave-packet dynamics in periodic potentials. Journal of Chemical Physics, 2003, 119, 5795-5804.	3.0	12
113	Influence of Nitroxide Spin Labels on RNA Structure: A Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2008, 4, 1781-1787.	5.3	12
114	Global Langevin model of multidimensional biomolecular dynamics. Journal of Chemical Physics, 2016, 145, 184114.	3.0	12
115	Vibrational energy transport in acetylbenzonitrile described by an ab initio-based quantum tier model. Chemical Physics, 2017, 482, 86-92.	1.9	11
116	Nonperturbative generalized master equation for the spin-boson problem. Physical Review E, 1995, 51, 3038-3044.	2.1	10
117	Data driven Langevin modeling of biomolecular dynamics. Journal of Chemical Physics, 2013, 138, 204106.	3.0	10
118	Photoinduced large amplitude motion as mechanism for pure electronic dephasing and its manifestation in continuousâ€wave and timeâ€resolved spectroscopy. Journal of Chemical Physics, 1994, 101, 246-254.	3.0	9
119	Classical phase-space analysis of vibronically coupled systems. Journal of Chemical Physics, 2002, 116, 69.	3.0	9
120	Classical Calculation of Transient Absorption Spectra Monitoring Ultrafast Electron Transfer Processes. Journal of Chemical Theory and Computation, 2006, 2, 1605-1617.	5.3	9
121	Reply to the comment on "Energy landscape of a small peptide revealed by dihedral angle principal component analysis― Proteins: Structure, Function and Bioinformatics, 2006, 64, 798-799.	2.6	9
122	Modeling non-Markovian data using Markov state and Langevin models. Journal of Chemical Physics, 2020, 153, 244112.	3.0	9
123	Data-Driven Langevin Modeling of Nonequilibrium Processes. Journal of Physical Chemistry B, 2021, 125, 8125-8136.	2.6	7
124	Cooperative Protein Allosteric Transition Mediated by a Fluctuating Transmission Network. Journal of Molecular Biology, 2022, 434, 167679.	4.2	7
125	Theoretical Description of Secondary Emission Reflecting Ultrafast Nonadiabatic Isomerizationâ€. Journal of Physical Chemistry A, 2001, 105, 2626-2633.	2.5	6
126	Classical description of the dynamics and time-resolved spectroscopy of nonadiabatic cis–trans photoisomerization. Chemical Physics, 2006, 329, 109-117.	1.9	6

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127	Simulation of transient infrared spectra of a photoswitchable peptide. Journal of Chemical Physics, 2011, 135, 225102.	3.0	6
128	Communication: Microsecond peptide dynamics from nanosecond trajectories: A Langevin approach. Journal of Chemical Physics, 2014, 141, 241102.	3.0	6
129	Mechanisms for allosteric activation of protease DegS by ligand binding and oligomerization as revealed from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1690-1705.	2.6	6
130	Molecular Origin of Driving-Dependent Friction in Fluids. Journal of Chemical Theory and Computation, 2022, 18, 2816-2825.	5.3	6
131	Periodic-Orbit Analysis of Coherent Electron-Transfer Femtosecond Experiments. Journal of Physical Chemistry A, 2002, 106, 8483-8487.	2.5	5
132	Improved Wang-Landau sampling through the use of smoothed potential-energy surfaces. Journal of Chemical Physics, 2006, 124, 154107.	3.0	5
133	Quantum modeling of transient infrared spectra reflecting photoinduced electron-transfer dynamics. Journal of Chemical Physics, 2006, 124, 114105.	3.0	4
134	EFFECT OF THE ION TREATMENT ON AN RNA HAIRPIN: MOLECULAR DYNAMICS STUDY. Indonesian Journal of Chemistry, 2012, 12, 1-11.	0.8	1
135	Cover Image, Volume 84, Issue 11. Proteins: Structure, Function and Bioinformatics, 2016, 84, C1.	2.6	0