Gerhard Stock

List of Publications by Year
in descending order

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135 papers	8,866 citations	44042 48 h-index	46771 89 g-index
140 all docs	140 docs citations	140 times ranked	5740 citing authors

#	Article	IF	Citations
1	Molecular Origin of Driving-Dependent Friction in Fluids. Journal of Chemical Theory and Computation, 2022, 18, 2816-2825.	2.3	6
2	Cooperative Protein Allosteric Transition Mediated by a Fluctuating Transmission Network. Journal of Molecular Biology, 2022, 434, 167679.	2.0	7
3	A Numerical Procedure to Evaluate Memory Effects in Nonâ€Equilibrium Coarseâ€Grained Models. Advanced Theory and Simulations, 2021, 4, 2000197.	1.3	22
4	Hierarchical dynamics in allostery following ATP hydrolysis monitored by single molecule FRET measurements and MD simulations. Chemical Science, 2021, 12, 3350-3359.	3.7	22
5	Through bonds or contacts? Mapping protein vibrational energy transfer using non-canonical amino acids. Nature Communications, 2021, 12, 3284.	5.8	28
6	Data-Driven Langevin Modeling of Nonequilibrium Processes. Journal of Physical Chemistry B, 2021, 125, 8125-8136.	1.2	7
7	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.	3.3	45
8	MSMPathfinder: Identification of Pathways in Markov State Models. Journal of Chemical Theory and Computation, 2020, 16, 7874-7882.	2.3	13
9	Multisecond ligand dissociation dynamics from atomistic simulations. Nature Communications, 2020, 11, 2918.	5.8	52
10	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	23.0	205
11	Master equation model to predict energy transport pathways in proteins. Journal of Chemical Physics, 2020, 152, 045103.	1.2	14
12	Modeling non-Markovian data using Markov state and Langevin models. Journal of Chemical Physics, 2020, 153, 244112.	1.2	9
13	Energy Transport Pathways in Proteins: A Non-equilibrium Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2019, 15, 5750-5757.	2.3	15
14	Photocontrolling Proteinâ€“Peptide Interactions: From Minimal Perturbation to Complete Unbinding. Journal of the American Chemical Society, 2019, 141, 10702-10710.	6.6	33
15	Principal component analysis of nonequilibrium molecular dynamics simulations. Journal of Chemical Physics, 2019, 150, 204110.	1.2	31
16	Dynamical coring of Markov state models. Journal of Chemical Physics, 2019, 150, 094111.	1.2	26
17	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
18	Machine Learning of Biomolecular Reaction Coordinates. Journal of Physical Chemistry Letters, 2018, 9, 2144-2150.	2.1	65

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19	Metadynamics Enhanced Markov Modeling of Protein Dynamics. Journal of Physical Chemistry B, 2018, 122, 5508-5514.	1.2	48
20	MELD-Path Efficiently Computes Conformational Transitions, Including Multiple and Diverse Paths. Journal of Chemical Theory and Computation, 2018, 14, 2109-2116.	2.3	13
21	Targeted Molecular Dynamics Calculations of Free Energy Profiles Using a Nonequilibrium Friction Correction. Journal of Chemical Theory and Computation, 2018, 14, 6175-6182.	2.3	41
22	Perspective: Identification of collective variables and metastable states of protein dynamics. Journal of Chemical Physics, 2018, 149, 150901.	1.2	105
23	Azidohomoalanine: A Minimally Invasive, Versatile, and Sensitive Infrared Label in Proteins To Study Ligand Binding. Journal of Physical Chemistry B, 2018, 122, 10118-10125.	1.2	18
24	A non-equilibrium approach to allosteric communication. Philosophical Transactions of the Royal Society B: Biological Sciences, 2018, 373, 20170187.	1.8	48
25	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.	2.3	35
26	Time-resolved observation of protein allosteric communication. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E6804-E6811.	3.3	63
27	2D-IR Spectroscopy of an AHA Labeled Photoswitchable PDZ2 Domain. Journal of Physical Chemistry A, 2017, 121, 9435-9445.	1.1	18
28	Vibrational energy transport in acetylbenzonitrile described by an ab initio-based quantum tier model. Chemical Physics, 2017, 482, 86-92.	0.9	11
29	Principal component analysis on a torus: Theory and application to protein dynamics. Journal of Chemical Physics, 2017, 147, 244101.	1.2	50
30	Global Langevin model of multidimensional biomolecular dynamics. Journal of Chemical Physics, 2016, 145, 184114.	1.2	12
31	Robust Density-Based Clustering To Identify Metastable Conformational States of Proteins. Journal of Chemical Theory and Computation, 2016, 12, 2426-2435.	2.3	68
32	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.	1.5	6
33	Cover Image, Volume 84, Issue 11. Proteins: Structure, Function and Bioinformatics, 2016, 84, C1.	1.5	0
34	Scaling Rules for Vibrational Energy Transport in Globular Proteins. Journal of Physical Chemistry Letters, 2016, 7, 25-30.	2.1	48
35	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.	2.3	23
36	Multidimensional Langevin Modeling of Nonoverdamped Dynamics. Physical Review Letters, 2015, 115, 050602.	2.9	20

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37	Nonadiabatic vibrational dynamics in the HCO2â˜â‹…H2O complex. Journal of Chemical Physics, 2015, 143, 134308.	1.2	20
38	Contact- and distance-based principal component analysis of protein dynamics. Journal of Chemical Physics, 2015, 143, 244114.	1.2	74
39	Vibrational energy flow in the villin headpiece subdomain: Master equation simulations. Journal of Chemical Physics, 2015, 142, 075101.	1.2	48
40	Hierarchical Biomolecular Dynamics: Picosecond Hydrogen Bonding Regulates Microsecond Conformational Transitions. Journal of Chemical Theory and Computation, 2015, 11, 1330-1336.	2.3	30
41	Inferring Transition Rates of Networks from Populations in Continuous-Time Markov Processes. Journal of Chemical Theory and Computation, 2015, 11, 5464-5472.	2.3	69
42	Principal component analysis of molecular dynamics: On the use of Cartesian vs. internal coordinates. Journal of Chemical Physics, 2014, 141, 014111.	1.2	149
43	Long-Range Conformational Transition of a Photoswitchable Allosteric Protein: Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 13468-13476.	1.2	26
44	Hierarchical Folding Free Energy Landscape of HP35 Revealed by Most Probable Path Clustering. Journal of Physical Chemistry B, 2014, 118, 7750-7760.	1.2	39
45	Communication: Microsecond peptide dynamics from nanosecond trajectories: A Langevin approach. Journal of Chemical Physics, 2014, 141, 241102.	1.2	6
46	Vibrational conical intersections in the water dimer. Molecular Physics, 2013, 111, 2046-2056.	0.8	22
47	Data driven Langevin modeling of biomolecular dynamics. Journal of Chemical Physics, 2013, 138, 204106.	1.2	10
48	Vibrational Conical Intersections as a Mechanism of Ultrafast Vibrational Relaxation. Physical Review Letters, 2012, 109, 173201.	2.9	38
49	Identifying Metastable States of Folding Proteins. Journal of Chemical Theory and Computation, 2012, 8, 3810-3819.	2.3	74
50	Construction of the Free Energy Landscape of Peptide Aggregation from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 1471-1479.	2.3	40
51	EFFECT OF THE ION TREATMENT ON AN RNA HAIRPIN: MOLECULAR DYNAMICS STUDY. Indonesian Journal of Chemistry, 2012, 12, 1-11.	0.3	1
52	Real Time Observation of Ultrafast Peptide Conformational Dynamics: Molecular Dynamics Simulation vs Infrared Experiment. Journal of Physical Chemistry B, 2011, 115, 13084-13092.	1.2	13
53	Simulation of transient infrared spectra of a photoswitchable peptide. Journal of Chemical Physics, 2011, 135, 225102.	1.2	6
54	Hidden Complexity of Protein Free-Energy Landscapes Revealed by Principal Component Analysis by Parts. Journal of Physical Chemistry Letters, 2010, 1, 2769-2773.	2.1	24

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55	Nonequilibrium molecular dynamics simulation of the energy transport through a peptide helix. Journal of Chemical Physics, 2010, 132, 025102.	1.2	66
56	Classical Simulation of Quantum Energy Flow in Biomolecules. Physical Review Letters, 2009, 102, 118301.	2.9	65
57	Multidimensional Langevin modeling of biomolecular dynamics. Journal of Chemical Physics, 2009, 130, 034106.	1.2	48
58	Molecular dynamics simulation of cooling: Heat transfer from a photoexcited peptide to the solvent. Journal of Chemical Physics, 2009, 131, 184503.	1.2	41
59	Quantum and classical vibrational relaxation dynamics of Nâ€methylacetamide on ab initio potential energy surfaces. International Journal of Quantum Chemistry, 2009, 109, 2047-2057.	1.0	22
60	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.	6.5	72
61	Energy Flow and Long-Range Correlations in Guanine-Binding Riboswitch: A Nonequilibrium Molecular Dynamics Study. Journal of Physical Chemistry B, 2009, 113, 9340-9347.	1.2	36
62	Free-Energy Landscape of RNA Hairpins Constructed via Dihedral Angle Principal Component Analysis. Journal of Physical Chemistry B, 2009, 113, 16660-16668.	1.2	53
63	Nonadiabatic vibrational dynamics and spectroscopy of peptides: A quantum-classical description. Chemical Physics, 2008, 347, 208-217.	0.9	24
64	Structural Flexibility of a Helical Peptide Regulates Vibrational Energy Transport Properties. Journal of Physical Chemistry B, 2008, 112, 15487-15492.	1.2	53
65	Maximum Caliber: A variational approach applied to two-state dynamics. Journal of Chemical Physics, 2008, 128, 194102.	1.2	49
66	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.	1.2	47
67	Energy Transport in Peptide Helices: A Comparison between High- and Low-Energy Excitations. Journal of Physical Chemistry B, 2008, 112, 9091-9099.	1.2	92
68	Influence of Nitroxide Spin Labels on RNA Structure: A Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2008, 4, 1781-1787.	2.3	12
69	NMR and MD studies of the temperature-dependent dynamics of RNA YNMG-tetraloops. Nucleic Acids Research, 2008, 36, 1928-1940.	6.5	56
70	Construction of the free energy landscape of biomolecules via dihedral angle principal component analysis. Journal of Chemical Physics, 2008, 128, 245102.	1.2	170
71	Dynamic treatment of vibrational energy relaxation in a heterogeneous and fluctuating environment. Journal of Chemical Physics, 2008, 129, 134110.	1.2	30
72	How Complex Is the Dynamics of Peptide Folding?. Physical Review Letters, 2007, 98, 028102.	2.9	85

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73	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.	3.3	344
74	Energy transport in peptide helices. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 12749-12754.	3.3	179
75	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.	6.6	304
76	Base-specific spin-labeling of RNA for structure determination. Nucleic Acids Research, 2007, 35, 3128-3143.	6.5	146
77	Dihedral angle principal component analysis of molecular dynamics simulations. Journal of Chemical Physics, 2007, 126, 244111.	1.2	279
78	Ab initio based building block model of amide I vibrations in peptides. Chemical Physics Letters, 2007, 437, 272-276.	1.2	33
79	Conformational Dynamics of RNA-Peptide Binding: A Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 90, 391-399.	0.2	35
80	Photoinduced Conformational Dynamics of a Photoswitchable Peptide: A Nonequilibrium Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 91, 1224-1234.	0.2	49
81	What NMR Relaxation Can Tell Us about the Internal Motion of an RNA Hairpin:â€‰ A Molecular Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2006, 2, 1228-1236.	2.3	39
82	Classical Calculation of Transient Absorption Spectra Monitoring Ultrafast Electron Transfer Processes. Journal of Chemical Theory and Computation, 2006, 2, 1605-1617.	2.3	9
83	Reply to the comment on â€œEnergy landscape of a small peptide revealed by dihedral angle principal component analysisâ€• Proteins: Structure, Function and Bioinformatics, 2006, 64, 798-799.	1.5	9
84	Classical description of the dynamics and time-resolved spectroscopy of nonadiabatic cisâ€“trans photoisomerization. Chemical Physics, 2006, 329, 109-117.	0.9	6
85	Nonequilibrium molecular dynamics simulation of a photoswitchable peptide. Chemical Physics, 2006, 323, 36-44.	0.9	60
86	Quantum modeling of transient infrared spectra reflecting photoinduced electron-transfer dynamics. Journal of Chemical Physics, 2006, 124, 114105.	1.2	4
87	Improved Wang-Landau sampling through the use of smoothed potential-energy surfaces. Journal of Chemical Physics, 2006, 124, 154107.	1.2	5
88	Modeling of decoherence and dissipation in nonadiabatic photoreactions by an effective-scaling nonsecular Redfield algorithm. Chemical Physics, 2005, 310, 33-41.	0.9	29
89	Structure and Dynamics of an RNA Tetraloop: A Joint Molecular Dynamics and NMR Study. Structure, 2005, 13, 1255-1267.	1.6	35
90	Structure and energy landscape of a photoswitchable peptide: A replica exchange molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 60, 485-494.	1.5	45

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91	Free energy landscape and folding mechanism of a Î²-hairpin in explicit water: A replica exchange molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 61, 795-808.	1.5	125
92	Ab initio-based exciton model of amide I vibrations in peptides: Definition, conformational dependence, and transferability. Journal of Chemical Physics, 2005, 122, 224904.	1.2	127
93	SYNTHESIS OF SPIN-LABELED RNAS FOR LONG RANGE DISTANCE MEASUREMENTS BY PELDOR. Nucleosides, Nucleotides and Nucleic Acids, 2005, 24, 771-775.	0.4	44
94	Energy landscape of a small peptide revealed by dihedral angle principal component analysis. Proteins: Structure, Function and Bioinformatics, 2004, 58, 45-52.	1.5	363
95	Transient Spectral Features of a cisâ^'trans Photoreaction in the Condensed Phase:â€‰ A Model Study. Journal of Physical Chemistry A, 2004, 108, 6464-6473.	1.1	18
96	A PELDOR-Based Nanometer Distance Ruler for Oligonucleotides. Journal of the American Chemical Society, 2004, 126, 5722-5729.	6.6	193
97	Mechanism of a photochemical funnel: a dissipative wave-packet dynamics study. Chemical Physics Letters, 2003, 379, 351-358.	1.2	45
98	Quasiclassical and semiclassical wave-packet dynamics in periodic potentials. Journal of Chemical Physics, 2003, 119, 5795-5804.	1.2	12
99	Nonequilibrium molecular-dynamics study of the vibrational energy relaxation of peptides in water. Journal of Chemical Physics, 2003, 119, 11350-11358.	1.2	80
100	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.	1.2	199
101	Quasiperiodic orbit analysis of nonadiabaticcisâ€“transphotoisomerization dynamics. Journal of Chemical Physics, 2003, 119, 4204-4215.	1.2	18
102	Ultrafastcis-transphotoswitching: A model study. Journal of Chemical Physics, 2002, 116, 1085-1091.	1.2	39
103	Classical phase-space analysis of vibronically coupled systems. Journal of Chemical Physics, 2002, 116, 69.	1.2	9
104	Peptide conformational heterogeneity revealed from nonlinear vibrational spectroscopy and molecular-dynamics simulations. Journal of Chemical Physics, 2002, 117, 6833-6840.	1.2	219
105	Conformational Dynamics of Trialanine in Water:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2002, 106, 5294-5301.	1.2	83
106	Periodic-Orbit Analysis of Coherent Electron-Transfer Femtosecond Experiments. Journal of Physical Chemistry A, 2002, 106, 8483-8487.	1.1	5
107	Efficient calculation of femtosecond time-resolved photoelectron spectra: method and application to the ionization of pyrazine. Physical Chemistry Chemical Physics, 2001, 3, 2331-2336.	1.3	27
108	Theoretical Description of Secondary Emission Reflecting Ultrafast Nonadiabatic Isomerizationâ€. Journal of Physical Chemistry A, 2001, 105, 2626-2633.	1.1	6

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109	Quantum-classical Liouville description of multidimensional nonadiabatic molecular dynamics. Journal of Chemical Physics, 2001, 114, 2001-2012.	1.2	79
110	Periodic Orbit Description of Nonadiabatic Quantum Dynamics. Physical Review Letters, 2001, 87, 140404.	2.9	12
111	Femtosecond secondary emission arising from the nonadiabatic photoisomerization in rhodopsin. Chemical Physics, 2000, 259, 297-312.	0.9	50
112	Semiclassical description of nonadiabatic quantum dynamics: Application to the S1â€“S2 conical intersection in pyrazine. Journal of Chemical Physics, 2000, 112, 10282-10292.	1.2	155
113	Approximate calculation of femtosecond pumpâ€“probe spectra monitoring nonadiabatic excited-state dynamics. Journal of Chemical Physics, 2000, 112, 4910-4922.	1.2	21
114	Quantum-Mechanical Modeling of the Femtosecond Isomerization in Rhodopsin. Journal of Physical Chemistry B, 2000, 104, 1146-1149.	1.2	151
115	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.	1.2	107
116	Mapping approach to the semiclassical description of nonadiabatic quantum dynamics. Physical Review A, 1999, 59, 64-79.	1.0	213
117	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.	1.2	117
118	Efficient calculation of time- and frequency-resolved spectra: a mixed non-perturbative/perturbative approach. Chemical Physics Letters, 1998, 296, 137-145.	1.2	16
119	Consistent treatment of quantum-mechanical and classical degrees of freedom in mixed quantum-classical simulations. Journal of Chemical Physics, 1998, 108, 7516-7526.	1.2	67
120	Surface-hopping modeling of photoinduced relaxation dynamics on coupled potential-energy surfaces. Journal of Chemical Physics, 1997, 107, 6230-6245.	1.2	239
121	Semiclassical Description of Nonadiabatic Quantum Dynamics. Physical Review Letters, 1997, 78, 578-581.	2.9	456
122	Femtosecond pump-probe spectroscopy of electron-transfer systems: a nonperturbative approach. Chemical Physics, 1997, 217, 275-287.	0.9	56
123	A semiclassical selfâ€consistentâ€field approach to dissipative dynamics. II. Internal conversion processes. Journal of Chemical Physics, 1995, 103, 2888-2902.	1.2	60
124	Nonperturbative generalized master equation for the spin-boson problem. Physical Review E, 1995, 51, 3038-3044.	0.8	10
125	Classical description of nonadiabatic photoisomerization processes and their realâ€time detection via femtosecond spectroscopy. Journal of Chemical Physics, 1995, 103, 10015-10029.	1.2	30
126	A semiclassical selfâ€consistentâ€field approach to dissipative dynamics: The spinâ€“boson problem. Journal of Chemical Physics, 1995, 103, 1561-1573.	1.2	100

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127	Resonance Raman spectroscopy of theS1andS2states of pyrazine: Experiment and first principles calculation of spectra. Journal of Chemical Physics, 1995, 103, 6851-6860.	1.2	81
128	Nonperturbative approach to femtosecond spectroscopy: General theory and application to multidimensional nonadiabatic photoisomerization processes. Journal of Chemical Physics, 1995, 103, 3998-4011.	1.2	197
129	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.	1.2	9
130	Classical description of ultrafast internal conversion processes. The benzene cation. Chemical Physics Letters, 1994, 224, 131-138.	1.2	21
131	Model studies on femtosecond spectroscopy of multidimensional photoisomerization and internal-conversion dynamics. A nonperturbative approach. Chemical Physics Letters, 1994, 228, 665-671.	1.2	19
132	Classical formulation of the spectroscopy of nonadiabatic excitedâ€state dynamics. Journal of Chemical Physics, 1993, 99, 1545-1555.	1.2	23
133	Detection of ultrafast molecular-excited-state dynamics with time- and frequency-resolved pump-probe spectroscopy. Physical Review A, 1992, 45, 3032-3040.	1.0	90
134	A classical model for time- and frequency-resolved spectroscopy of nonadiabatic excited-state dynamics. Chemical Physics Letters, 1992, 197, 396-404.	1.2	20
135	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.	1.2	15