Klaus B MÃ¸ller

List of Publications by Year
in descending order

97 papers	3,244 citations	126907 33 h-index	161849 54 g-index
101 all docs	101 docs citations	101 times ranked	2864 citing authors

#	Article	IF	Citations
1	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy. Journal of Physical Chemistry A, 2002, 106, 11993-11996.	2.5	325
2	Hydrogen Bond Dynamics in Water and Ultrafast Infrared Spectroscopy:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 1275-1289.	2.5	252
3	Ultrafast Vibrational Population Dynamics of Water and Related Systems:Â A Theoretical Perspective. Chemical Reviews, 2004, 104, 1915-1928.	47.7	163
4	Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses. Nature Communications, 2015, 6, 6359.	12.8	134
5	Finding intersections between electronic excited state potential energy surfaces with simultaneous ultrafast X-ray scattering and spectroscopy. Chemical Science, 2019, 10, 5749-5760.	7.4	90
6	Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo stretchy="false">[</mml:mo><mml:mi>Co</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mtext) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 532 Td (mathvariant="bold">terpy</mml:mtext><mml:	7.8	86
7	Observing Solvation Dynamics with Simultaneous Femtosecond X-ray Emission Spectroscopy and X-ray Scattering. Journal of Physical Chemistry B, 2016, 120, 1158-1168.	2.6	85
8	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. Nature Communications, 2020, 11, 634.	12.8	75
9	Atomistic characterization of the active-site solvation dynamics of a model photocatalyst. Nature Communications, 2016, 7, 13678.	12.8	74
10	Detailed Characterization of a Nanosecond-Lived Excited State: X-ray and Theoretical Investigation of the Quintet State in Photoexcited [Fe(terpy)₂]²⁺. Journal of Physical Chemistry C, 2015, 119, 5888-5902.	3.1	72
11	On the Theory of Time-Resolved X-ray Diffraction. Journal of Physical Chemistry B, 2008, 112, 558-567.	2.6	65
12	Ultrafast X-Ray Scattering Measurements of Coherent Structural Dynamics on the Ground-State Potential Energy Surface of a Diplatinum Molecule. Physical Review Letters, 2019, 122, 063001.	7.8	64
13	Interpretation of the Ultrafast Photoinduced Processes in Pentacene Thin Films. Journal of the American Chemical Society, 2010, 132, 3431-3439.	13.7	59
14	Filming the Birth of Molecules and Accompanying Solvent Rearrangement. Journal of the American Chemical Society, 2013, 135, 3255-3261.	13.7	59
15	Between ethylene and polyenes - the non-adiabatic dynamics of cis-dienes. Faraday Discussions, 2012, 157, 193.	3.2	54
16	Quantum dynamics for dissipative systems: A hydrodynamic perspective. Journal of Chemical Physics, 2002, 117, 7409-7425.	3.0	50
17	Displaced squeezed number states: Position space representation, inner product, and some applications. Physical Review A, 1996, 54, 5378-5385.	2.5	49
18	Toward Highlighting the Ultrafast Electron Transfer Dynamics at the Optically Dark Sites of Photocatalysts. Journal of Physical Chemistry Letters, 2013, 4, 1972-1976.	4.6	49

#	ARTICLE	IF	CITATIONS
19	Solution Structure and Ultrafast Vibrational Relaxation of the PtPOP Complex Revealed by Î”SCF-QM/MM Direct Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 7100-7119.	3.1	46
20	On the interpretation of time-resolved anisotropic diffraction patterns. New Journal of Physics, 2010, 12, 113022.	2.9	45
21	On the coupling between molecular diffusion and solvation shell exchange. Journal of Chemical Physics, 2005, 122, 114508.	3.0	43
22	Electronic Coherence in Ultrafast X-Ray Scattering from Molecular Wave Packets. Physical Review Letters, 2019, 122, 073003.	7.8	41
23	Hot Branching Dynamics in a Lightâ€Harvesting Iron Carbene Complex Revealed by Ultrafast Xâ€ray Emission Spectroscopy. Angewandte Chemie - International Edition, 2020, 59, 364-372.	13.8	41
24	On coherent-state representations of quantum mechanics: Wave mechanics in phase space. Journal of Chemical Physics, 1997, 106, 7228-7240.	3.0	40
25	Direct Dynamics Studies of a Binuclear Metal Complex in Solution: The Interplay Between Vibrational Relaxation, Coherence, and Solvent Effects. Journal of Physical Chemistry Letters, 2014, 5, 2414-2418.	4.6	39
26	On the role of coherence in the transition from kinetics to dynamics: Theory and application to femtosecond unimolecular reactions. Journal of Chemical Physics, 2000, 113, 10477-10485.	3.0	37
27	Effect of tert-Butyl Functionalization on the Photoexcited Decay of a Fe(II)-N-Heterocyclic Carbene Complex. Journal of Physical Chemistry C, 2016, 120, 17234-17241.	3.1	37
28	Ultrafast Librational Relaxation of H₂O in Liquid Water. Journal of Physical Chemistry B, 2013, 117, 4541-4552.	2.6	35
29	Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations. Physical Chemistry Chemical Physics, 2014, 16, 11770-11779.	2.8	35
30	Wave packet dynamics and photofragmentation in timeâ€dependent quadratic potentials. Journal of Chemical Physics, 1996, 105, 5037-5047.	3.0	34
31	New insights on the photodynamics of acetone excited with 253â”288nm femtosecond pulses. Chemical Physics Letters, 2008, 461, 193-197.	2.6	34
32	On the calculation of x-ray scattering signals from pairwise radial distribution functions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 244010.	1.5	34
33	Butterfly Deformation Modes in a Photoexcited Pyrazolate-Bridged Pt Complex Measured by Time-Resolved X-Ray Scattering in Solution. Journal of Physical Chemistry A, 2016, 120, 7475-7483.	2.5	34
34	The Nonâ€Ergodic Nature of Internal Conversion. ChemPhysChem, 2014, 15, 249-259.	2.1	33
35	Anisotropy enhanced X-ray scattering from solvated transition metal complexes. Journal of Synchrotron Radiation, 2018, 25, 306-315.	2.4	33
36	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. Journal of Chemical Theory and Computation, 2017, 13, 6010-6022.	5.3	32

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37	Time-resolved near-edge X-ray absorption fine structure of pyrazine from electronic structure and nuclear wave packet dynamics simulations. Journal of Chemical Physics, 2019, 151, 124114.	3.0	32
38	Theory of time-resolved inelastic x-ray diffraction. Physical Review A, 2010, 81, .	2.5	30
39	Time-Resolved X-Ray Diffraction: The Dynamics of the Chemical Bond. Structure and Bonding, 2011, , 185-211.	1.0	29
40	Theoretical Evidence of Solvent-Mediated Excited-State Dynamics in a Functionalized Iron Sensitizer. Journal of Physical Chemistry C, 2019, 123, 2056-2065.	3.1	29
41	X-ray transient absorption reveals the 1Au (nÏ€*) state of pyrazine in electronic relaxation. Nature Communications, 2021, 12, 5003.	12.8	29
42	Coherent Motion Reveals Nonâ€Ergodic Nature of Internal Conversion between Excited States. ChemPhysChem, 2012, 13, 820-827.	2.1	28
43	Femtosecond dynamics of transition states: the classical saddle-point barrier reactions. Chemical Physics Letters, 1998, 295, 1-10.	2.6	24
44	Theory of ultrafast x-ray scattering by molecules in the gas phase. Journal of Chemical Physics, 2019, 151, 174302.	3.0	24
45	Wigner Method Dynamics in the Interaction Picture. The Journal of Physical Chemistry, 1994, 98, 3272-3279.	2.9	20
46	Probing spinâ€“vibronic dynamics using femtosecond X-ray spectroscopy. Faraday Discussions, 2016, 194, 731-746.	3.2	20
47	Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation. Angewandte Chemie - International Edition, 2013, 52, 2247-2250.	13.8	19
48	Simulation of ultrafast excited-state dynamics and elastic x-ray scattering by quantum wavepacket dynamics. Journal of Chemical Physics, 2019, 151, 104307.	3.0	19
49	Mechanism of Photoinduced Dihydroazulene Ring-Opening Reaction. Journal of Physical Chemistry Letters, 2019, 10, 3944-3949.	4.6	19
50	Quantum control fields from instantaneous dynamics. Chemical Physics Letters, 2004, 398, 180-185.	2.6	18
51	Selective bond breakage within the HOD molecule using optimized femtosecond ultraviolet laser pulses. Physical Review A, 2008, 78, .	2.5	18
52	Initial Dynamics of The Norrish Type I Reaction in Acetone: Probing Wave Packet Motion. Journal of Physical Chemistry A, 2011, 115, 556-561.	2.5	18
53	An assessment of different electronic structure approaches for modeling time-resolved x-ray absorption spectroscopy. Structural Dynamics, 2021, 8, 024101.	2.3	18
54	Theoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffraction. Journal of Physical Chemistry A, 2008, 112, 8179-8187.	2.5	17

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55	Symmetry, vibrational energy redistribution and vibronic coupling: The internal conversion processes of cycloketones. Journal of Chemical Physics, 2012, 137, 22A522.	3.0	17
56	Quantum hydrodynamics: Mixed states, dissipation, and a new hybrid quantum-classical approach. International Journal of Quantum Chemistry, 2004, 100, 1153-1162.	2.0	16
57	Real-Time Probing of Structural Dynamics by Interaction between Chromophores. Journal of Physical Chemistry A, 2011, 115, 12120-12125.	2.5	16
58	Electron Transfer and Solvent-Mediated Electronic Localization in Molecular Photocatalysis. Inorganic Chemistry, 2016, 55, 10637-10644.	4.0	16
59	Time-resolved X-ray scattering by electronic wave packets: analytic solutions to the hydrogen atom. Physical Chemistry Chemical Physics, 2017, 19, 19740-19749.	2.8	16
60	Isotope effects in the photofragmentation of symmetric molecules: The branching ratio of ODâ•OH in water. Journal of Chemical Physics, 2005, 122, 204320.	3.0	15
61	How To Excite Nuclear Wavepackets into Electronically Degenerate States in Spin-Vibronic Quantum Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3967-3974.	5.3	15
62	Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods. Physical Chemistry Chemical Physics, 2019, 21, 4082-4095.	2.8	15
63	Hot Branching Dynamics in a Lightâ€Harvesting Iron Carbene Complex Revealed by Ultrafast Xâ€ray Emission Spectroscopy. Angewandte Chemie, 2020, 132, 372-380.	2.0	14
64	Kinetics modeling of dynamics: the case of femtosecond-activated direct reactions. Chemical Physics Letters, 2002, 351, 281-288.	2.6	13
65	Selective bond breakage in HOD with shaped UV-femtosecond laser pulses. Chemical Physics Letters, 2006, 419, 65-69.	2.6	13
66	Instantaneous nonvertical electronic transitions with shaped femtosecond laser pulses: Is it possible?. Journal of Chemical Physics, 2003, 119, 2569-2576.	3.0	12
67	Approaches to Wave Packet Imaging Using Femtosecond Ionization Spectroscopyâ€. Journal of Physical Chemistry A, 2004, 108, 8954-8960.	2.5	12
68	Charge-resonance excitations in symmetric molecules â€“ Comparison of linear response DFT with CC3 for the excited states of a model dimer. Chemical Physics Letters, 2009, 478, 127-131.	2.6	11
69	Resolving Femtosecond Solvent Reorganization Dynamics in an Iron Complex by Nonadiabatic Dynamics Simulations. Journal of the American Chemical Society, 2022, 144, 12861-12873.	13.7	11
70	Comment on â€œTheoretical Investigation of Perylene Dimers and Excimers and Their Signatures in X-Ray Diffractionâ€. Journal of Physical Chemistry A, 2009, 113, 6849-6850.	2.5	10
71	Validity of the Bersohnâ€“Zewail model beyond justification. Chemical Physics Letters, 2012, 539-540, 234-238.	2.6	10
72	Solvent-Controlled Chemoselectivity in the Photolytic Release of Hydroxamic Acids and Carboxamides from Solid Support. Organic Letters, 2017, 19, 3263-3266.	4.6	10

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73	Ultrafast structural dynamics of photo-reactions observed by time-resolved x-ray cross-correlation analysis. Structural Dynamics, 2019, 6, 024301.	2.3	10
74	Intrinsic resonance representation of quantum mechanics. Journal of Chemical Physics, 1997, 106, 8564-8571.	3.0	9
75	Femtosecond Activation of Reactions: The Concepts of Nonergodic Behavior and Reduced-Space Dynamics. , 0, , 157-188.		9
76	Wave Packet Simulation of Nonadiabatic Dynamics in Highly Excited 1,3-Dibromopropane. Journal of Physical Chemistry A, 2008, 112, 10481-10486.	2.5	9
77	Characterizing the Solvated Structure of Photoexcited [Os(terpy)2]2+ with X-ray Transient Absorption Spectroscopy and DFT Calculations. Molecules, 2016, 21, 235.	3.8	9
78	Azobenzene photoisomerization dynamics: Revealing the key degrees of freedom and the long timescale of the trans-to-cis process. Journal of Photochemistry and Photobiology A: Chemistry, 2022, 428, 113869.	3.9	9
79	Theoretical Investigation on the Control of Macrocyclic Dihydroazulene/Azobenzene Photoswitches. Journal of Physical Chemistry C, 2019, 123, 25579-25584.	3.1	7
80	Comment on phase-space representation of quantum state vectors. Journal of Mathematical Physics, 1999, 40, 2531-2535.	1.1	5
81	Suppressing the Spreading of Continuum Wave Packets via Chirped Laser Pulsesâ€. Journal of Physical Chemistry A, 2004, 108, 8840-8847.	2.5	5
82	Controlling the spreading of wave packets of a dissociating molecule. Chemical Physics Letters, 2007, 450, 6-11.	2.6	5
83	Elucidating the Ultrafast Dynamics of Photoinduced Charge Separation in Metalloporphyrin-Fullerene Dyads Across the Electromagnetic Spectrum. Journal of Physical Chemistry C, 2016, 120, 19537-19546.	3.1	5
84	Trajectory surface-hopping photoinduced dynamics from Rydberg states of trimethylamine. Physical Chemistry Chemical Physics, 2021, 23, 10964-10977.	2.8	5
85	Role that separatrices and stochastic webs play in quantum dynamics. Physical Review A, 1998, 57, 771-780.	2.5	4
86	The concept of coherent resonances in the nuclear motion of bimolecular collisions: femtosecond probing and the classical picture. Chemical Physics Letters, 1999, 309, 1-13.	2.6	3
87	Perspective: Preservation of coherence in photophysical processes. Structural Dynamics, 2018, 5, 060901.	2.3	3
88	Ultrafast non-Franckâ€“Condon transitions via a two-pulse scheme. Chemical Physics Letters, 2004, 385, 134-139.	2.6	2
89	Ultrafast X-ray absorption study of longitudinalâ€“transverse phonon coupling in electrolyte aqueous solution. Physical Chemistry Chemical Physics, 2017, 19, 27266-27274.	2.8	2
90	On ultrafast IR spectroscopy in water. , 2004, , 177-180.		2

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91	On wave-packet dynamics in a decaying quadratic potential. Physica Scripta, 1997, 55, 542-546.	2.5	1
92	Ultrafast Rotational and Translational Energy Relaxation in Neat Liquids. Journal of Physical Chemistry B, 2021, 125, 12806-12819.	2.6	1
93	Femtochemistry of bimolecular reactions from weakly bound complexes: computational study of the H + Hâ€²OD â†' Hâ€²OH + D or HOD + Hâ€² exchange reactions. Physical Chemistry Chemical Physics, 2021, 23, 27207-27226.	2.8	1
94	RÃ¼cktitelbild: Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation (Angew. Chem. 8/2013). Angewandte Chemie, 2013, 125, 2432-2432.	2.0	0
95	Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone. EPJ Web of Conferences, 2013, 41, 02033.	0.3	0
96	Ultrafast non-Franck-Condon transitions: is it possible?. , 2004, , 135-138.		0
97	Time-resolved photoelectron spectroscopy and ab initio multiple spawning studies of hexamethylcyclopentadiene. , 2014, , .		0