

# Markus Gerhards

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6581814/publications.pdf>

Version: 2024-02-01

86  
papers

2,536  
citations

172457

29  
h-index

223800

46  
g-index

89  
all docs

89  
docs citations

89  
times ranked

1728  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structure of a $\beta$ -sheet model system in the gas phase: Analysis of the C=O stretching vibrations. Physical Chemistry Chemical Physics, 2002, 4, 5563-5565.	2.8	120
2	$\beta$ -sheet model systems in the gas phase: Structures and vibrations of Ac-Phe-NHMe and its dimer (Ac-Phe-NHMe) <sub>2</sub> . Physical Chemistry Chemical Physics, 2004, 6, 2682-2690.	2.8	102
3	Deuterated Molecular Ruby with Record Luminescence Quantum Yield. Angewandte Chemie - International Edition, 2018, 57, 1112-1116.	13.8	94
4	Structures of the protected amino acid Ac-Phe-OMe and its dimer: A $\beta$ -sheet model system in the gas phase. Physical Chemistry Chemical Physics, 2002, 4, 1760-1765.	2.8	88
5	Luminescence and Light-Driven Energy and Electron Transfer from an Exceptionally Long-Lived Excited State of a Non-Innocent Chromium(III) Complex. Angewandte Chemie - International Edition, 2019, 58, 18075-18085.	13.8	87
6	Infrared Spectroscopy of Resonantly Ionized (Phenol)(H <sub>2</sub> O) <sub>n</sub> <sup>+</sup> . Journal of Physical Chemistry A, 1999, 103, 5232-5239.	2.5	86
7	A Vanadium(III) Complex with Blue and NIR-II Spin-Flip Luminescence in Solution. Journal of the American Chemical Society, 2020, 142, 7947-7955.	13.7	74
8	High energy and narrow bandwidth mid IR nanosecond laser system. Optics Communications, 2004, 241, 493-497.	2.1	72
9	Ultraviolet/infrared-double resonance spectroscopy and ab initio calculations on the indole <sup>+</sup> and indole(H <sub>2</sub> O) <sub>1</sub> <sup>+</sup> cations. Journal of Chemical Physics, 2000, 113, 7945-7954.	3.0	71
10	Structure of the protected dipeptide Ac-Val-Phe-OMe in the gas phase: Towards a $\beta$ -sheet model system. Journal of Chemical Physics, 2003, 118, 8296-8300.	3.0	69
11	Strongly Red-Emissive Molecular Ruby [Cr(bmp) <sub>2</sub> ] <sup>3+</sup> Surpasses [Ru(bpy) <sub>3</sub> ] <sup>2+</sup> . Journal of the American Chemical Society, 2021, 143, 11843-11855.	13.7	66
12	Investigation of Secondary Structure Elements by IR/UV Double Resonance Spectroscopy: Analysis of an Isolated $\beta$ -Sheet Model System. Journal of the American Chemical Society, 2008, 130, 4692-4698.	13.7	61
13	OH stretching vibrations in aromatic cations: IR/PIRL spectroscopy. Chemical Physics Letters, 1998, 297, 515-522.	2.6	59
14	Investigations on isolated peptides by combined IR/UV spectroscopy in a molecular beam - structure, aggregation, solvation and molecular recognition. International Reviews in Physical Chemistry, 2016, 35, 569-677.	2.3	51
15	Structure of the tripeptide model Ac-Val-Tyr(Me)-NHMe and its cluster with water investigated by IR/UV double resonance spectroscopy. Physical Chemistry Chemical Physics, 2004, 6, 4636-4641.	2.8	50
16	Structure and vibrations of catechol in the S <sub>1</sub> state and ionic ground state. Chemical Physics Letters, 1998, 294, 65-70.	2.6	49
17	Towards Printed Organic Light-Emitting Devices: A Solution-Stable, Highly Soluble Cu <sup>I</sup> -NHetPHOS. Chemistry - A European Journal, 2016, 22, 16400-16405.	3.3	48
18	New Hexanuclear Group-11 Pyrazolate Complexes: Synthesis and Photophysical Features. Chemistry - A European Journal, 2011, 17, 3384-3389.	3.3	46

#	ARTICLE	IF	CITATIONS
19	Nâ€Heterocyclic Carbene Complexes of Iron as Photosensitizers for Lightâ€Induced Water Reduction. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 1504-1509.	2.0	46
20	Structure of a Î²-sheet model system in the gas phase: Analysis of the fingerprint region up to 10 Åµm. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1660.	2.8	45
21	IR double-resonance spectroscopy applied to the 4-aminophenol(H <sub>2</sub> O) <sub>1</sub> cluster. <i>Applied Physics A: Materials Science and Processing</i> , 2001, 72, 273-279.	2.3	44
22	Transient IR spectroscopy and ab initio calculations on ESIPT in 3-hydroxyflavone solvated in acetonitrile. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15007.	2.8	43
23	Neutral Peptides in the Gas Phase: Conformation and Aggregation Issues. <i>Chemical Reviews</i> , 2020, 120, 12490-12562.	47.7	40
24	Investigations of the water clusters of the protected amino acid Ac-Phe-OMe by applying IR/UV double resonance spectroscopy: microsolvation of the backbone. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3511.	2.8	36
25	Structural Analysis of an Isolated Cyclic Tetrapeptide and its Monohydrate by Combined IR/UV Spectroscopy. <i>ChemPhysChem</i> , 2011, 12, 1981-1988.	2.1	36
26	Spectroscopic, Structural, and Kinetic Investigation of the Ultrafast Spin Crossover in an Unusual Cobalt(II) Semiquinonate Radical Complex. <i>Chemistry - A European Journal</i> , 2017, 23, 2119-2132.	3.3	36
27	Remarkable high efficiency of red emitters using Eu(III) ternary complexes. <i>Chemical Communications</i> , 2018, 54, 5221-5224.	4.1	36
28	Structures and rearrangement reactions of 4-aminophenol(H <sub>2</sub> O) <sub>1+</sub> and 3-aminophenol(H <sub>2</sub> O) <sub>1+</sub> clusters. <i>Journal of Chemical Physics</i> , 2005, 123, 074320.	3.0	34
29	IR/UV spectroscopy on jet cooled 3-hydroxyflavone (H <sub>2</sub> O) <sub>n</sub> (n=1,2) clusters along proton transfer coordinates in the electronic ground and excited states. <i>Journal of Chemical Physics</i> , 2008, 129, 234306.	3.0	32
30	Infrared/ultraviolet quadruple resonance spectroscopy to investigate structures of electronically excited states. <i>Journal of Chemical Physics</i> , 2012, 136, 114202.	3.0	30
31	IR spectroscopy applied subsequent to a proton transfer reaction in the excited state of isolated 3-hydroxyflavone and 2-(2-naphthyl)-3-hydroxychromone. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1173.	2.8	29
32	Ultrafast and long-time excited state kinetics of an NIR-emissive vanadium(III) complex I: synthesis, spectroscopy and static quantum chemistry. <i>Chemical Science</i> , 2021, 12, 10780-10790.	7.4	28
33	Aromatic embedding wins over classical hydrogen bonding â€“ a multi-spectroscopic approach for the diphenyl etherâ€“methanol complex. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25975-25983.	2.8	27
34	Double resonance spectroscopy of different conformers of the neurotransmitter amphetamine and its clusters with water. <i>Chemical Physics</i> , 2006, 327, 43-53.	1.9	26
35	Luminescence and Lightâ€Driven Energy and Electron Transfer from an Exceptionally Longâ€Lived Excited State of a Nonâ€Innocent Chromium(III) Complex. <i>Angewandte Chemie</i> , 2019, 131, 18243-18253.	2.0	26
36	Secondary structure binding motifs of the jet cooled tetrapeptide model Acâ€“Leuâ€“Valâ€“Tyr(Me)â€“NHMe. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 4592.	2.8	25

#	ARTICLE	IF	CITATIONS
37	Highly soluble fluorine containing Cu( <i>i</i> ) AlkylPyrPhos TADF complexes. Dalton Transactions, 2019, 48, 15687-15698.	3.3	25
38	Investigation of Luminescent Triplet States in Tetranuclear Cu <sup>I</sup> Complexes: Thermochromism and Structural Characterization. Chemistry - A European Journal, 2021, 27, 5439-5452.	3.3	25
39	Structures of Ac <sup>+</sup> Trp <sup>+</sup> OMe and its dimer (Ac <sup>+</sup> Trp <sup>+</sup> OMe) <sub>2</sub> in the gas phase: influence of a polar group in the side-chain. Molecular Physics, 2005, 103, 1521-1529.	1.7	24
40	Chromium(0) and Molybdenum(0) Complexes with a Pyridyl-Mesoionic Carbene Ligand: Structural, (Spectro)electrochemical, Photochemical, and Theoretical Investigations. Inorganic Chemistry, 2020, 59, 15504-15513.	4.0	24
41	Time-resolved IR spectroscopy of a trinuclear palladium complex in solution. Physical Chemistry Chemical Physics, 2015, 17, 14138-14144.	2.8	23
42	Photophysical dynamics of a binuclear Cu( <i>i</i> )-emitter on the fs to 1/4s timescale, in solid phase and in solution. Physical Chemistry Chemical Physics, 2017, 19, 29438-29448.	2.8	23
43	Spin Crossover and Long-Lived Excited States in a Reduced Molecular Ruby. Chemistry - A European Journal, 2020, 26, 7199-7204.	3.3	23
44	NIR-Emissive Chromium(0), Molybdenum(0), and Tungsten(0) Complexes in the Solid State at Room Temperature. Chemistry - A European Journal, 2021, 27, 12959-12964.	3.3	22
45	Deutrierter molekularer Rubin mit Rekord-Lumineszenzquantenausbeute. Angewandte Chemie, 2018, 130, 1125-1130.	2.0	21
46	Dispersion-controlled docking preference: multi-spectroscopic study on complexes of dibenzofuran with alcohols and water. Physical Chemistry Chemical Physics, 2019, 21, 16032-16046.	2.8	21
47	Clusters of a protected amino acid with pyrazole derivatives: -sheet model systems in the gas phase. European Physical Journal D, 2002, 20, 543-550.	1.3	20
48	Structure of Isolated Xanthone in the T <sub>1</sub> State Obtained via Combined UV/IR Spectroscopy. ChemPhysChem, 2009, 10, 1882-1886.	2.1	20
49	Infrared and electronic absorption spectra as well as ultrafast spin dynamics in isolated $\text{Co}^{3+}$		

#	ARTICLE	IF	CITATIONS
55	Comprehensive Picture of the Excited State Dynamics of Cu(I)- and Ru(II)-Based Photosensitizers with Long-Lived Triplet States. <i>Inorganic Chemistry</i> , 2022, 61, 214-226.	4.0	15
56	Structural investigations on a linear isolated depsipeptide: the importance of dispersion interactions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15327-15336.	2.8	14
57	Characterization of the isolated [Co <sub>3</sub> Ni(EtOH)] <sup>+</sup> cluster by IR spectroscopy and spin-dynamics calculations. <i>Physical Review B</i> , 2018, 97, .	3.2	14
58	Thermally Activated Delayed Fluorescence and Phosphorescence Quenching in Iminophosphonamide Copper and Zinc Complexes. <i>Chemistry - A European Journal</i> , 2021, 27, 15110-15119.	3.3	14
59	Time-Resolved Spectroscopy and Electronic Structure of Mono- and Dinuclear Pyridyl-Triazole/DPEPhos-Based Cu(I) Complexes. <i>Chemistry - A European Journal</i> , 2021, 27, 15252-15271.	3.3	14
60	Real-time observation of molecular flattening and intersystem crossing in [(DPEPhos)Cu( <i>scpi</i> )(PyrTet)] <i>via</i> ultrafast UV/Vis- and mid-IR spectroscopy on solution and solid samples. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14187-14200.	2.8	13
61	Dispersion-Bound Isolated Dimers in the Gas Phase: Observation of the Shortest Intermolecular CH...H <sup>+</sup> C Distance via Stimulated Raman Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 11305-11309.	13.8	13
62	Solid-State Step-Scan FTIR Spectroscopy of Binuclear Copper(I) Complexes. <i>ChemPhysChem</i> , 2017, 18, 3023-3029.	2.1	12
63	The phenyl vinyl ether-methanol complex: a model system for quantum chemistry benchmarking. <i>Beilstein Journal of Organic Chemistry</i> , 2018, 14, 1642-1654.	2.2	12
64	Transient FTIR spectroscopy after one- and two-colour excitation on a highly luminescent chromium( <i>scpiii</i> ) complex. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13808-13818.	2.8	12
65	A combined IR/IR and IR/UV spectroscopy study on the proton transfer coordinate of isolated 3-hydroxychromone in the electronic ground and excited state. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21795-21803.	2.8	11
66	In-depth exploration of the photophysics of a trinuclear palladium complex. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8332-8338.	2.8	10
67	Control of Cooperativity through a Reversible Structural Phase Transition in MoMethyl/Cu(111). <i>Advanced Functional Materials</i> , 2018, 28, 1703544.	14.9	10
68	Proton/Hydrogen-Transfer Coordinate of 2,5-Dihydroxybenzoic Acid Investigated in a Supersonic Beam: Combined IR/UV Spectroscopy in the S <sub>0</sub> , S <sub>1</sub> , and D <sub>0</sub> States. <i>ChemPhysChem</i> , 2008, 9, 2592-2600.	2.1	9
69	The Structure of Diphenyl Ether-Methanol in the Electronically Excited and Ionic Ground States: A Combined IR/UV Spectroscopic and Theoretical Study. <i>ChemPhysChem</i> , 2017, 18, 3634-3641.	2.1	9
70	Structural analyses of isolated cyclic tetrapeptides with varying amino acid residues. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10718-10726.	2.8	8
71	An intermolecular C-H oxidizing strategy to access highly fused carbazole skeletons from simple naphthylamines. <i>Chemical Communications</i> , 2019, 55, 13749-13752.	4.1	8
72	Quantification of Cooperativity between Metal Sites in Dinuclear Transition Metal Complexes Containing the (2-Dimethylamino)-4-(2-pyrimidinyl)pyrimidine Ligand. <i>ChemPlusChem</i> , 2021, 86, 622-628.	2.8	8

#	ARTICLE	IF	CITATIONS
73	Structures and internal dynamics of diphenylether and its aggregates with water. Physical Chemistry Chemical Physics, 2020, 22, 27966-27978.	2.8	7
74	Investigation of the hydrated 7-hydroxy-4-methylcoumarin dimer by combined IR/UV spectroscopy. Journal of Chemical Physics, 2014, 141, 194304.	3.0	6
75	IR and IR + UV spectroscopy of isolated [Al <sup>+</sup> AcPheOMe] <sub>n</sub> cluster cations (n = 1, 3). Physical Chemistry Chemical Physics, 2012, 14, 8185.	2.8	5
76	Photoemission Studies on Na <sup>+</sup> -Substituted Dithienylated Phenothiazines. ChemPhysChem, 2015, 16, 1996-2005.	2.1	5
77	Playing with Pearson's concept: orthogonally functionalized 1,4-diaza-1,3-butadienes leading to heterobinuclear complexes. Dalton Transactions, 2018, 47, 9643-9656.	3.3	5
78	Der Effekt von Dispersionswechselwirkungen auf die Struktur von Diphenylether-Ä aggregaten. Angewandte Chemie, 2018, 130, 9678-9682.	2.0	4
79	Structural Characterization and Lifetimes of Triple-Stranded Helical Coinage Metal Complexes: Synthesis, Spectroscopy and Quantum Chemical Calculations. Chemistry - A European Journal, 2020, 26, 10743-10751.	3.3	3
80	Structural Rearrangement by Isomer-Specific Infrared Excitation in the Neutral Isolated Dihydrated Cluster of 3-Hydroxyflavone. Journal of Physical Chemistry Letters, 2018, 9, 4360-4366.	4.6	2
81	Synthesis and photophysical properties of multimetallic gold/zinc complexes of (P,N,N,N,P) and (P,N,N) ligands. New Journal of Chemistry, 2022, 46, 4062-4071.	2.8	2
82	Frontispiece: Towards Printed Organic Light-Emitting Devices: A Solution-Stable, Highly Soluble Cu <sup>I</sup> -NHetPHOS. Chemistry - A European Journal, 2016, 22, .	3.3	0
83	A Phosphino-Carboxylic Acid-Based Ru Dimeric Complex. European Journal of Inorganic Chemistry, 2018, 2018, 1394-1398.	2.0	0
84	Titelbild: Luminescence and Light-Driven Energy and Electron Transfer from an Exceptionally Long-Lived Excited State of a Non-Innocent Chromium(III) Complex (Angew. Chem. 50/2019). Angewandte Chemie, 2019, 131, 18045-18045.	2.0	0
85	Dispersionsgebundene, isolierte Dimere in der Gasphase: Beobachtung des kürzesten intermolekularen C-H...H-Abstands mittels stimulierter Raman-Spektroskopie. Angewandte Chemie, 2021, 133, 11405-11410.	2.0	0
86	Chromone-methanol clusters in the electronic ground and lowest triplet state: a delicate interplay of non-covalent interactions. Physical Chemistry Chemical Physics, 2022, , .	2.8	0