

# Stephan Kupfer

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5472344/publications.pdf>

Version: 2024-02-01

92  
papers

1,794  
citations

218381

26  
h-index

329751

37  
g-index

98  
all docs

98  
docs citations

98  
times ranked

2070  
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards synthetic unimolecular [Fe <sub>2</sub> S <sub>2</sub> ]-photocatalysts sensitized by perylene dyes. Dyes and Pigments, 2022, 198, 109940.	2.0	7
2	A Highly Fluorescent Dinuclear Aluminium Complex with Near-Unity Quantum Yield**. Angewandte Chemie - International Edition, 2022, 61, .	7.2	10
3	Active repair of a dinuclear photocatalyst for visible-light-driven hydrogen production. Nature Chemistry, 2022, 14, 500-506.	6.6	32
4	Light-Driven Multi-Charge Separation in a Push-Pull Ruthenium-Based Photosensitizer – Assessed by RASSCF and TDDFT Simulations. ChemPhotoChem, 2022, 6, .	1.5	4
5	Activating a [FeFe] Hydrogenase Mimic for Hydrogen Evolution under Visible Light**. Angewandte Chemie - International Edition, 2022, , .	7.2	6
6	A Combined Spectroscopic and Theoretical Study on a Ruthenium Complex Featuring a –Extended dppz Ligand for Light-Driven Accumulation of Multiple Reducing Equivalents. Chemistry - A European Journal, 2022, 28, e202103882.	1.7	5
7	Ligand-Induced Donor State Destabilisation – A New Route to Panchromatically Absorbing Cu(I) Complexes. Chemistry - A European Journal, 2022, , .	1.7	5
8	Co-facial – – Interaction Expedites Sensitizer-to-Catalyst Electron Transfer for High-Performance CO <sub>2</sub> Photoreduction. JACS, 2022, 144, 1359-1374.	3.6	24
9	Unravelling the Mystery: Enlightenment of the Uncommon Electrochemistry of Naphthalene Monoimide [FeFe] Hydrogenase Mimics. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	6
10	Novel [FeFe]-Hydrogenase Mimics: Unexpected Course of the Reaction of Ferrocenyl –-Thienyl Thioketone with Fe <sub>3</sub> (CO) <sub>12</sub> . Materials, 2022, 15, 2867.	1.3	7
11	Deep-Red Luminescent Molybdenum(0) Complexes with –-and Tridentate Isocyanide Chelate Ligands. ChemPhotoChem, 2022, 6, .	1.5	9
12	Frontispiz: Aktivierung eines biomimetischen [FeFe]-Hydrogenase-Komplexes für die H <sub>2</sub> -Produktion mit sichtbarem Licht. Angewandte Chemie, 2022, 134, .	1.6	0
13	Frontispiece: Activating a [FeFe] Hydrogenase Mimic for Hydrogen Evolution under Visible Light. Angewandte Chemie - International Edition, 2022, 61, .	7.2	0
14	Metal-ligand bonding in tricarbonyliron(0) complexes bearing thiochalcone ligands. New Journal of Chemistry, 2022, 46, 12924-12933.	1.4	1
15	Reaction Mechanism of Pd-Catalyzed –CO-Free-Carbonylation Reaction Uncovered by In Situ Spectroscopy: The Formyl Mechanism. Angewandte Chemie - International Edition, 2021, 60, 3422-3427.	7.2	9
16	pysisyphus: Exploring potential energy surfaces in ground and excited states. International Journal of Quantum Chemistry, 2021, 121, e26390.	1.0	29
17	Photochlorination of toluene – the thin line between intensification and selectivity. Part 2: selectivity. Reaction Chemistry and Engineering, 2021, 6, 90-99.	1.9	11
18	Excitation Energy-Dependent Branching Dynamics Determines Photostability of Iron(II)-Mesoionic Carbene Complexes. Inorganic Chemistry, 2021, 60, 9157-9173.	1.9	15

#	ARTICLE	IF	CITATIONS
19	Excited-State Switching in Rhenium(I) Bipyridyl Complexes with Donor–Donor and Donor–Acceptor Substituents. <i>Journal of the American Chemical Society</i> , 2021, 143, 9082-9093.	6.6	19
20	Chemical Enhancement vs Molecule–Substrate Geometry in Plasmon-Enhanced Spectroscopy. <i>ACS Photonics</i> , 2021, 8, 2243-2255.	3.2	16
21	Tuning the metal–ligand bond in the $\sigma$ -complexes of stannylenes and azabenzenes. <i>Journal of Computational Chemistry</i> , 2021, 42, 2103-2115.	1.5	2
22	Covalent Linkage of BODIPY–Photosensitizers to Anderson–Type Polyoxometalates Using CLICK Chemistry. <i>Chemistry - A European Journal</i> , 2021, 27, 17181-17187.	1.7	13
23	New insights into the biphasic $\text{CO-free}$ Pauson–Khand cyclisation reaction through combined <i>in situ</i> spectroscopy and multiple linear regression modelling. <i>Catalysis Science and Technology</i> , 2021, 11, 1626-1636.	2.1	1
24	Are charged tips driving TERS-resolution? A full quantum chemical approach. <i>Journal of Chemical Physics</i> , 2021, 154, 034106.	1.2	13
25	<i>Z</i> -Selective phosphine promoted 1,4-reduction of $\alpha$ -keto esters and propynoic amides in the presence of water. <i>Organic and Biomolecular Chemistry</i> , 2021, 19, 6092-6097.	1.5	9
26	Hydrogen Production at a NiO Photocathode Based on a Ruthenium Dye–Cobalt Diimine Dioxime Catalyst Assembly: Insights from Advanced Spectroscopy and Post-operando Characterization. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 49802-49815.	4.0	16
27	A Molecular Photosensitizer in a Porous Block Copolymer Matrix—Implications for the Design of Photocatalytically Active Membranes. <i>Chemistry - A European Journal</i> , 2021, 27, 17049-17058.	1.7	6
28	Modulating the Excited-State Decay Pathways of Cu(I) 4-H-Imidazolates Complexes by Excitation Wavelength and Ligand Backbone. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11498-11511.	1.2	5
29	Coupling of photoactive transition metal complexes to a functional polymer matrix**. <i>Chemistry - A European Journal</i> , 2021, 27, 17104-17114.	1.7	5
30	Role of MLCT States in the Franck–Condon Region of Neutral, Heteroleptic Cu(I) 4-H-imidazolates Complexes: A Spectroscopic and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6607-6616.	1.1	13
31	Tetraaryl Cyclopentadienones: Experimental and Theoretical Insights into Negative Solvatochromism and Electrochemistry. <i>European Journal of Organic Chemistry</i> , 2020, 2020, 6555-6562.	1.2	3
32	Molecular Scylla and Charybdis: Maneuvering between pH Sensitivity and Excited-State Localization in Ruthenium Bi(benz)imidazole Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 12097-12110.	1.9	19
33	Iron(0)-Mediated Stereoselective (3+2)-Cycloaddition of Thiochalcones via a Diradical Intermediate. <i>Chemistry - A European Journal</i> , 2020, 26, 11412-11416.	1.7	8
34	The chemical effect goes resonant – a full quantum mechanical approach on TERS. <i>Nanoscale</i> , 2020, 12, 6346-6359.	2.8	29
35	Excited-State Switching Frustrates the Tuning of Properties in Triphenylamine-Donor-Ligand Ruthenium(I) and Platinum(II) Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 6736-6746.	1.9	16
36	The role of anchoring groups in ruthenium(II)-bipyridine sensitized p-type semiconductor solar cells—a quantum chemical approach. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 234001.	0.6	3

#	ARTICLE	IF	CITATIONS
37	Frontispiece: Two-Photon-Induced CO-Releasing Molecules as Molecular Logic Systems in Solution, Polymers, and Cells. <i>Chemistry - A European Journal</i> , 2019, 25, .	1.7	0
38	Unraveling the Light-Activated Reaction Mechanism in a Catalytically Competent Key Intermediate of a Multifunctional Molecular Catalyst for Artificial Photosynthesis. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 13140-13148.	7.2	34
39	Metal-Free Aryl Cross-Coupling Directed by Traceless Linkers. <i>Chemistry - A European Journal</i> , 2019, 25, 16068-16073.	1.7	11
40	Unraveling the Light-Activated Reaction Mechanism in a Catalytically Competent Key Intermediate of a Multifunctional Molecular Catalyst for Artificial Photosynthesis. <i>Angewandte Chemie</i> , 2019, 131, 13274-13282.	1.6	9
41	Effect of the Catalytic Center on the Electron Transfer Dynamics in Hydrogen-Evolving Ruthenium-Based Photocatalysts Investigated by Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16003-16013.	1.5	15
42	Visible light-activated biocompatible photo-CORM for CO-release with colorimetric and fluorometric dual turn-on response. <i>Polyhedron</i> , 2019, 172, 175-181.	1.0	10
43	Two-Photon-Induced CO-Releasing Molecules as Molecular Logic Systems in Solution, Polymers, and Cells. <i>Chemistry - A European Journal</i> , 2019, 25, 8453-8458.	1.7	15
44	Excited state properties of a series of molecular photocatalysts investigated by time dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 9052-9060.	1.3	12
45	Resonance Raman Spectro-Electrochemistry to Illuminate Photo-Induced Molecular Reaction Pathways. <i>Molecules</i> , 2019, 24, 245.	1.7	9
46	A SERS-based molecular sensor for selective detection and quantification of copper(II) ions. <i>Sensors and Actuators B: Chemical</i> , 2019, 279, 230-237.	4.0	51
47	Hydrogel-Embedded Model Photocatalytic System Investigated by Raman and IR Spectroscopy Assisted by Density Functional Theory Calculations and Two-Dimensional Correlation Analysis. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2677-2687.	1.1	7
48	Sterically induced distortions of nickel(II) porphyrins – Comprehensive investigation by DFT calculations and resonance Raman spectroscopy. <i>Coordination Chemistry Reviews</i> , 2018, 360, 1-16.	9.5	35
49	Fate of Photoexcited Molecular Antennae - Intermolecular Energy Transfer versus Photodegradation Assessed by Quantum Dynamics. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3273-3285.	1.5	6
50	Unusually Short-Lived Solvent-Dependent Excited State in a Half-Sandwich Ru(II) Complex Induced by Low-Lying $\pi^*$ MC States. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1550-1559.	1.1	2
51	A $\pi^*$ State Enables Photoaccumulation of Charges on a $\pi$ -Extended Dipyridophenazine Ligand in a Ru(II) Polypyridine Complex. <i>Journal of Physical Chemistry C</i> , 2018, 122, 83-95.	1.5	19
52	An artificial photosynthetic system for photoaccumulation of two electrons on a fused dipyridophenazine (dppz)-pyridoquinolinone ligand. <i>Chemical Science</i> , 2018, 9, 4152-4159.	3.7	48
53	Dramatic Alteration of $\pi$ -ILCT Lifetimes Using Ancillary Ligands in $[\text{Re}(\text{L})(\text{CO})_3(\text{phen-TPA})]^{+}$ Complexes: An Integrated Spectroscopic and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2018, 140, 4534-4542.	6.6	49
54	Highly fluorescent single crystals of a 4-ethoxy-1,3-thiazole. <i>Dyes and Pigments</i> , 2018, 149, 644-651.	2.0	9

#	ARTICLE	IF	CITATIONS
55	Photo-Induced Charge Separation vs. Degradation of a BODIPY-Based Photosensitizer Assessed by TDDFT and RASPT2. <i>Catalysts</i> , 2018, 8, 520.	1.6	11
56	Cu( <i>vs.</i> ) Ru photosensitizers: elucidation of electron transfer processes within a series of structurally related complexes containing an extended $\pi$ -system. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24843-24857.	1.3	50
57	Theoretical Investigation of the Electron Transfer Dynamics and Photodegradation Pathways in a Hydrogen-Evolving Ruthenium-Palladium Photocatalyst. <i>Chemistry - A European Journal</i> , 2018, 24, 11166-11176.	1.7	12
58	Photophysics of a Ruthenium Complex with a $\pi$ -Extended Dipyridophenazine Ligand for DNA Quadruplex Labeling. <i>Journal of Physical Chemistry A</i> , 2018, 122, 6558-6569.	1.1	10
59	Theoretical Assessment of Excited State Gradients and Resonance Raman Intensities for the Azobenzene Molecule. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1263-1274.	2.3	26
60	Intrinsic self-healing polymers with a high E-modulus based on dynamic reversible urea bonds. <i>NPG Asia Materials</i> , 2017, 9, e420-e420.	3.8	97
61	Light-responsive paper strips as CO-releasing material with a colourimetric response. <i>Chemical Science</i> , 2017, 8, 6555-6560.	3.7	23
62	Photochemistry and Electron Transfer Kinetics in a Photocatalyst Model Assessed by Marcus Theory and Quantum Dynamics. <i>Journal of Physical Chemistry C</i> , 2017, 121, 16066-16078.	1.5	35
63	[FeFe]-Hydrogenase H-cluster mimics mediated by naphthalene monoimide derivatives of peri-substituted dichalcogenides. <i>Dalton Transactions</i> , 2017, 46, 11180-11191.	1.6	43
64	Photophysics of BODIPY Dyes as Readily-Designable Photosensitisers in Light-Driven Proton Reduction. <i>Inorganics</i> , 2017, 5, 21.	1.2	25
65	Extended charge accumulation in ruthenium-4H-imidazole-based black absorbers: a theoretical design concept. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 13357-13367.	1.3	13
66	Spatial resolution of tip-enhanced Raman spectroscopy – DFT assessment of the chemical effect. <i>Nanoscale</i> , 2016, 8, 10229-10239.	2.8	64
67	Spectroelectrochemical Investigation of the One-Electron Reduction of Nonplanar Nickel(II) Porphyrins. <i>ChemPhysChem</i> , 2016, 17, 3480-3493.	1.0	8
68	Synthesis of three series of ruthenium tris-diimine complexes containing acridine-based $\pi$ -extended ligands using an efficient $\sigma$ -chemistry on the complex approach. <i>Dalton Transactions</i> , 2016, 45, 16298-16308.	1.6	10
69	Influence of Protonation State on the Excited State Dynamics of a Photobiologically Active Ru(II) Dyad. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6379-6388.	1.1	29
70	Sensitization of NO-Releasing Ruthenium Complexes to Visible Light. <i>Chemistry - A European Journal</i> , 2015, 21, 15554-15563.	1.7	14
71	Synthesis and Characterization of Ga <sup>III</sup> , In <sup>III</sup> and Lu <sup>III</sup> Complexes of a Set of dtpa Bis-Amide Ligands. <i>European Journal of Inorganic Chemistry</i> , 2015, 2015, 4125-4137.	1.0	5
72	The Self-Healing Potential of Triazole-Pyridine-Based Metallopolymers. <i>Macromolecular Rapid Communications</i> , 2015, 36, 604-609.	2.0	37

#	ARTICLE	IF	CITATIONS
73	Photophysics of a Ruthenium 4 <i>H</i> -imidazole Panchromatic Dye in Interaction with Titanium Dioxide. <i>ChemPhysChem</i> , 2015, 16, 1061-1070.	1.0	14
74	Ultrafast Intramolecular Relaxation and Wavepacket Motion in a Ruthenium-Based Supramolecular Photocatalyst. <i>Chemistry - A European Journal</i> , 2015, 21, 7668-7674.	1.7	24
75	Photophysics of Ru(II) Dyads Derived from Pyrenyl-Substituted Imidazo[4,5- <i>f</i> ][1,10]phenanthroline Ligands. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3986-3994.	1.1	34
76	In situ spectroelectrochemical and theoretical study on the oxidation of a 4 <i>H</i> -imidazole-ruthenium dye adsorbed on nanocrystalline TiO <sub>2</sub> thin film electrodes. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29637-29646.	1.3	16
77	And yet they glow: thiazole based push-pull fluorophores containing nitro groups and the influence of regioisomerism. <i>Methods and Applications in Fluorescence</i> , 2015, 3, 025005.	1.1	16
78	Trapped in Imidazole: How to Accumulate Multiple Photoelectrons on a Black-Absorbing Ruthenium Complex. <i>Chemistry - A European Journal</i> , 2014, 20, 3793-3799.	1.7	38
79	Resonance-Raman spectro-electrochemistry of intermediates in molecular artificial photosynthesis of bimetallic complexes. <i>Chemical Communications</i> , 2014, 50, 5227.	2.2	48
80	Self-healing mechanism of metallopolymers investigated by QM/MM simulations and Raman spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12422.	1.3	53
81	Tuning of photocatalytic activity by creating a tridentate coordination sphere for palladium. <i>Dalton Transactions</i> , 2014, 43, 11676.	1.6	23
82	Synthesis, properties and quantum chemical evaluation of solvatochromic pyridinium-phenyl-1,3-thiazol-4-olate betaine dyes. <i>Tetrahedron</i> , 2013, 69, 1489-1498.	1.0	12
83	An Assessment of RASSCF and TDDFT Energies and Gradients on an Organic Donor-Acceptor Dye Assisted by Resonance Raman Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 543-554.	2.3	38
84	Structural Control of Photoinduced Dynamics in 4 <i>H</i> -Imidazole-Ruthenium Dyes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25664-25676.	1.5	38
85	Arylamine-Modified Thiazoles as Donor-Acceptor Dyes: Quantum Chemical Evaluation of the Charge-Transfer Process and Testing as Ligands in Ruthenium(II) Complexes. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 5231-5247.	1.2	26
86	A Novel Ru(II) Polypyridine Black Dye Investigated by Resonance Raman Spectroscopy and TDDFT Calculations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 19968-19977.	1.5	30
87	Singlet oxygen generation versus O <sup>1</sup> O homolysis in phenyl-substituted anthracene endoperoxides investigated by RASPT2, CASPT2, CC2, and TD-DFT methods. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	5
88	4-Methoxy-1,3-thiazole based donor-acceptor dyes: Characterization, X-ray structure, DFT calculations and test as sensitizers for DSSC. <i>Dyes and Pigments</i> , 2012, 94, 512-524.	2.0	67
89	Influence of Multiple Protonation on the Initial Excitation in a Black Dye. <i>Journal of Physical Chemistry C</i> , 2011, 115, 24004-24012.	1.5	28
90	Protonation effects on the resonance Raman properties of a novel (terpyridine)Ru(4 <i>H</i> -imidazole) complex: an experimental and theoretical case study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 15580.	1.3	54

#	ARTICLE	IF	CITATIONS
91	A Highly Fluorescent Dinuclear Aluminium Complex with Near-Unity Quantum Yield. Angewandte Chemie, 0, , .	1.6	0
92	Aktivierung eines biomimetischen [FeFe]-Hydrogenase-Komplexes für die H <sub>2</sub> -Produktion mit sichtbarem Licht**. Angewandte Chemie, 0, , .	1.6	0