Petter Persson

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1244801/publications.pdf

Version: 2024-02-01

117 papers	7,280 citations	44069 48 h-index	54911 84 g-index
120 all docs	120 docs citations	120 times ranked	6732 citing authors

#	Article	IF	Citations
1	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. Nature, 2002, 418, 620-623.	27.8	346
2	Quantum Chemical Study of Photoinjection Processes in Dye-Sensitized TiO2Nanoparticles. Journal of Physical Chemistry B, 2000, 104, 10348-10351.	2.6	333
3	A low-spin Fe(iii) complex with 100-ps ligand-to-metal charge transfer photoluminescence. Nature, 2017, 543, 695-699.	27.8	287
4	Ultrafast Electron Dynamics in Solar Energy Conversion. Chemical Reviews, 2017, 117, 10940-11024.	47.7	266
5	Quantum Chemical Calculations of the Influence of Anchor-Cum-Spacer Groups on Femtosecond Electron Transfer Times in Dye-Sensitized Semiconductor Nanocrystals. Journal of Chemical Theory and Computation, 2006, 2, 441-451.	5.3	249
6	Luminescence and reactivity of a charge-transfer excited iron complex with nanosecond lifetime. Science, 2019, 363, 249-253.	12.6	249
7	DFT study of bare and dye-sensitized TiO2 clusters and nanocrystals. International Journal of Quantum Chemistry, 2006, 106, 3214-3234.	2.0	230
8	A 3.0 Î¼s Room Temperature Excited State Lifetime of a Bistridentate Ruâ^'Polypyridine Complex for Rod-like Molecular Arrays. Journal of the American Chemical Society, 2006, 128, 12616-12617.	13.7	203
9	Fe N-Heterocyclic Carbene Complexes as Promising Photosensitizers. Accounts of Chemical Research, 2016, 49, 1477-1485.	15.6	197
10	Iron sensitizer converts light to electrons with 92% yield. Nature Chemistry, 2015, 7, 883-889.	13.6	193
11	Calculated Structural and Electronic Interactions of the Ruthenium Dye N3 with a Titanium Dioxide Nanocrystal. Journal of Physical Chemistry B, 2005, 109, 11918-11924.	2.6	181
12	Bistridentate Ruthenium(II)polypyridyl-Type Complexes with Microsecond ³MLCT State Lifetimes: Sensitizers for Rod-Like Molecular Arrays. Journal of the American Chemical Society, 2008, 130, 15533-15542.	13.7	177
13	Adsorption of bi-isonicotinic acid on rutile TiO2(110). Journal of Chemical Physics, 1999, 110, 5913-5918.	3.0	165
14	Phosphonic acid adsorption at the TiO2 anatase (101) surface investigated by periodic hybrid HF-DFT computations. Surface Science, 2005, 582, 49-60.	1.9	163
15	Fe^{II} Hexa N-Heterocyclic Carbene Complex with a 528 ps Metal-to-Ligand Charge-Transfer Excited-State Lifetime. Journal of Physical Chemistry Letters, 2018, 9, 459-463.	4.6	151
16	Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts. Journal of Physical Chemistry C, 2008, 112, 14645-14654.	3.1	138
17	Anchor group influence on moleculeâ€“metal oxide interfaces: Periodic hybrid DFT study of pyridine bound to TiO2 via carboxylic and phosphonic acid. Chemical Physics Letters, 2005, 415, 375-380.	2.6	137
18	A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3â€triazolâ€5â€ylidene) Ligands: Taming the MLCT Excited State of Iron(II). Chemistry - A European Journal, 2015, 21, 3628-3639.	3.3	132

#	Article	IF	Citations
19	Steric Influence on the Excited-State Lifetimes of Ruthenium Complexes with Bipyridylâˆ’Alkanyleneâˆ’Pyridyl Ligands. Inorganic Chemistry, 2008, 47, 3540-3548.	4.0	127
20	Exceptional Excited-State Lifetime of an Iron(II)â€“N-Heterocyclic Carbene Complex Explained. Journal of Physical Chemistry Letters, 2014, 5, 2066-2071.	4.6	125
21	Spacer and Anchor Effects on the Electronic Coupling in Ruthenium-bis-Terpyridine Dye-Sensitized TiO2Nanocrystals Studied by DFT. Journal of Physical Chemistry B, 2006, 110, 20513-20525.	2.6	115
22	PES Studies of Ru(dcbpyH2)2(NCS)2Adsorption on Nanostructured ZnO for Solar Cell Applications. Journal of Physical Chemistry B, 2002, 106, 10102-10107.	2.6	106
23	The electronic structure and reflectivity of PEDOT:PSS from density functional theory. Chemical Physics, 2011, 384, 44-51.	1.9	102
24	Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution. Chemical Science, 2017, 8, 515-523.	7.4	102
25	Development of the ReaxFF reactive force field for mechanistic studies of catalytic selective oxidation processes on BiMoO x. Topics in Catalysis, 2006, 38, 93.	2.8	98
26	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. Langmuir, 2013, 29, 7838-7846.	3.5	96
27	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
28	XPS studies of Ru-polypyridine complexes for solar cell applications. Journal of Chemical Physics, 1999, 111, 2744-2750.	3.0	88
29	Dye-Sensitization of the TiO₂ Rutile (110) Surface by Perylene Dyes:â€‰ Quantum-Chemical Periodic B3LYP Computations. Journal of Physical Chemistry C, 2007, 111, 12116-12123.	3.1	84
30	Influence of Triplet State Multidimensionality on Excited State Lifetimes of Bis-tridentate Ru^{II} Complexes: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 1041-1050.	2.5	84
31	Dâ€“A₁â€“Dâ€“A₂ Copolymers with Extended Donor Segments for Efficient Polymer Solar Cells. Macromolecules, 2015, 48, 1009-1016.	4.8	82
32	Dynamical Simulation of Photoinduced Electron Transfer Reactions in Dyeâˆ’Semiconductor Systems with Different Anchor Groups. Journal of Physical Chemistry C, 2008, 112, 12326-12333.	3.1	81
33	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. Nature Communications, 2020, 11, 634.	12.8	75
34	Nâ€Š1s x-ray absorption study of the bonding interaction of bi-isonicotinic acid adsorbed on rutile TiO2(110). Journal of Chemical Physics, 2000, 112, 3945-3948.	3.0	68
35	The Smallest Possible Nanocrystals of Semiionic Oxides. Journal of Physical Chemistry B, 2003, 107, 3336-3339.	2.6	68
36	Periodic Hartreeâ€“Fock study of the adsorption of formic acid on ZnO(1010). Chemical Physics Letters, 2000, 321, 302-308.	2.6	63

#	Article	IF	Citations
37	Synthesis and Electron Transfer Studies of Rutheniumâ^'Terpyridine-Based Dyads Attached to Nanostructured TiO2. Inorganic Chemistry, 2007, 46, 638-651.	4.0	63
38	Electronic interactions between aromatic adsorbates and metal oxide substrates calculated from first principles. Chemical Physics Letters, 2002, 364, 469-474.	2.6	60
39	Theoretical Study of the Fast Photodissociation Channels of the Monohalobenzenes. Journal of Physical Chemistry A, 2004, 108, 2339-2345.	2.5	59
40	Computational Study of the Lowest Triplet State of Ruthenium Polypyridyl Complexes Used in Artificial Photosynthesis. Journal of Physical Chemistry A, 2008, 112, 4470-4476.	2.5	58
41	Cyclometallated Iridium and Platinum Complexes with Noninnocent Ligands. Inorganic Chemistry, 2007, 46, 3865-3875.	4.0	57
42	Structural study of adsorption of isonicotinic acid and related molecules on rutile TiO2(110) I: XAS and STM. Surface Science, 2003, 540, 39-54.	1.9	52
43	Solvent control of charge transfer excited state relaxation pathways in [Fe(2,2â€²-bipyridine)(CN)₄]^{2â^'}. Physical Chemistry Chemical Physics, 2018, 20, 4238-4249.	2.8	52
44	Photophysics and Photochemistry of Iron Carbene Complexes for Solar Energy Conversion and Photocatalysis. Catalysts, 2020, 10, 315.	3.5	52
45	Periodic INDO calculations of organic adsorbates on a TiO2 surface. International Journal of Quantum Chemistry, 1998, 70, 1055-1066.	2.0	51
46	Binding of bi-isonicotinic acid to anatase TiO2 (101). Solar Energy Materials and Solar Cells, 2000, 63, 139-148.	6.2	50
47	Microsecond Photoluminescence and Photoreactivity of a Metal-Centered Excited State in a Hexacarbeneâ€"Co(III) Complex. Journal of the American Chemical Society, 2021, 143, 1307-1312.	13.7	50
48	Tracking the picosecond deactivation dynamics of a photoexcited iron carbene complex by time-resolved X-ray scattering. Chemical Science, 2018, 9, 405-414.	7.4	49
49	Photodissociation of bromobenzene, dibromobenzene, and 1,3,5-tribromobenzene. Journal of Chemical Physics, 2004, 120, 6502-6509.	3.0	44
50	Photofunctionality of iron(III) N-heterocyclic carbenes and related d transition metal complexes. Coordination Chemistry Reviews, 2021, 426, 213517.	18.8	44
51	Quantum chemical prediction of the adsorption conformations and dynamics at HCOOH-covered ZnO(1010) surfaces. International Journal of Quantum Chemistry, 2002, 89, 172-180.	2.0	41
52	Photoinduced electron transfer processes in dye-semiconductor systems with different spacer groups. Journal of Chemical Physics, 2012, 137, 22A529.	3.0	41
53	Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2â€²-bipyridine)2(CN)2]. Structural Dynamics, 2017, 4, 044030.	2.3	41
54	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

#	Article	IF	Citations
55	Tuning the Electronics of Bis(tridentate)ruthenium(II) Complexes with Long-Lived Excited States: Modifications to the Ligand Skeleton beyond Classical Electron Donor or Electron Withdrawing Group Decorations. Inorganic Chemistry, 2013, 52, 5128-5137.	4.0	40
56	Photochemistry of Bromofluorobenzenes. Journal of Physical Chemistry A, 2006, 110, 7045-7056.	2.5	36
57	Shake-up and shake-off excitations with associated electron losses in X-ray studies of proteins. Protein Science, 2009, 10, 2480-2484.	7.6	36
58	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. ChemSusChem, 2016, 9, 667-675.	6.8	36
59	Bi-isonicotinic acid on rutile (110): calculated molecular and electronic structure. Surface Science, 2003, 529, 47-58.	1.9	35
60	Tracing the Full Bimolecular Photocycle of Iron(III)â€“Carbene Light Harvesters in Electron-Donating Solvents. Journal of the American Chemical Society, 2020, 142, 8565-8569.	13.7	34
61	Highâ€Performance Hole Transport and Quasiâ€Balanced Ambipolar OFETs Based on Dâ€“Aâ€“A Thienoâ€benzoâ€isoindigo Polymers. Advanced Electronic Materials, 2016, 2, 1500313.	5.1	32
62	Calculated Optoelectronic Properties of Ruthenium Tris-bipyridine Dyes Containing Oligophenyleneethynylene Rigid Rod Linkers in Different Chemical Environments. Journal of Physical Chemistry A, 2007, 111, 1487-1497.	2.5	30
63	Excited state potential energy surfaces of bistridentate RuII complexes â€“ A TD-DFT study. Chemical Physics, 2012, 407, 76-82.	1.9	29
64	Emerging polymorphism in nanostructured TiO₂ : Quantum chemical comparison of anatase, rutile, and brookite clusters. International Journal of Quantum Chemistry, 2013, 113, 2611-2620.	2.0	29
65	Light-harvesting capabilities of low band gap donorâ€“acceptor polymers. Physical Chemistry Chemical Physics, 2014, 16, 24853-24865.	2.8	28
66	Multireference calculations of the phosphorescence and photodissociation of chlorobenzene. Journal of Chemical Physics, 2004, 121, 11000.	3.0	27
67	Frequency dispersed transient absorption spectra of dissolved perylene: A case study using the density matrix version of the MCTDH method. Chemical Physics, 2008, 347, 152-165.	1.9	27
68	Orbital Topology Controlling Charge Injection in Quantum-Dot-Sensitized Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 1157-1162.	4.6	27
69	One-Step Synthesis of Precursor Oligomers for Organic Photovoltaics: A Comparative Study between Polymers and Small Molecules. ACS Applied Materials & Interfaces, 2015, 7, 27106-27114.	8.0	25
70	Calculations of interfacial interactions in pyrene-Ipa rod sensitized nanostructured TiO2. Dalton Transactions, 2009, , 10021.	3.3	23
71	Quantum Chemical Calculations of Side-Group Stacking and Electronic Properties in Thiopheneâ€“Quinoxaline Polymers. Journal of Physical Chemistry C, 2012, 116, 26700-26706.	3.1	23
72	Large Footprint Pyrene Chromophores Anchored to Planar and Colloidal Metal Oxide Thin Films. Langmuir, 2009, 25, 9219-9226.	3.5	21

#	Article	IF	Citations
73	A Stable Homoleptic Organometallic Iron(IV) Complex. Chemistry - A European Journal, 2020, 26, 12728-12732.	3.3	21
74	Electron dynamics within Ru-2,2â€²-bipyridine complexesâ€”an N1s core level excitation study. Chemical Physics, 2002, 285, 167-176.	1.9	18
75	Structures of Tetrafluorocyclopropene, Hexafluorocyclobutene, Octafluorocyclopentene and Related Perfluoroalkene Radical Anions Revealed by Electron Spin Resonance Spectroscopic and Computational Studies. Journal of Physical Chemistry A, 2006, 110, 6307-6323.	2.5	18
76	Temperature-Dependent Optical Properties of Flexible Donorâ€“Acceptor Polymers. Journal of Physical Chemistry C, 2015, 119, 6453-6463.	3.1	17
77	Dye-sensitized solar cells based on Fe N-heterocyclic carbene photosensitizers with improved rod-like push-pull functionality. Chemical Science, 2021, 12, 16035-16053.	7.4	17
78	Siteâ€selective participator decay of coreâ€excited butadiene. Journal of Chemical Physics, 1996, 105, 10719-10724.	3.0	15
79	Triarylamine on Nanocrystalline TiO2 Studied in Its Reduced and Oxidized State by Photoelectron Spectroscopy. Journal of Physical Chemistry B, 2001, 105, 7182-7187.	2.6	14
80	Defining donor and acceptor strength in conjugated copolymers. Molecular Physics, 2017, 115, 485-496.	1.7	14
81	Electronic structure and excited state properties of iron carbene photosensitizers â€“ A combined X-ray absorption and quantum chemical investigation. Chemical Physics Letters, 2017, 683, 559-566.	2.6	14
82	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
83	On the excited-state multi-dimensionality in cyanines. Chemical Physics Letters, 2008, 455, 13-19.	2.6	12
84	Meta-substituted RuII rigid rods for sensitization of TiO2. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 206, 155-163.	3.9	12
85	Rational design of Dâ€“A₁â€“Dâ€“A₂ conjugated polymers with superior spectral coverage. Physical Chemistry Chemical Physics, 2015, 17, 26677-26689.	2.8	12
86	Band-selective dynamics in charge-transfer excited iron carbene complexes. Faraday Discussions, 2019, 216, 191-210.	3.2	12
87	Site-Selective Orbital Interactions in an Ultrathin Iron-Carbene Photosensitizer Film. Journal of Physical Chemistry A, 2020, 124, 1603-1609.	2.5	12
88	Theoretical study of the photodissociation of low lying excited states of hydrogen peroxide. Molecular Physics, 2004, 102, 2575-2584.	1.7	11
89	Conformation sensitive charge transport in conjugated polymers. Applied Physics Letters, 2013, 103, 213303.	3.3	11
90	Exploring Photoinduced Excited State Evolution in Heterobimetallic Ru(II)â€“Co(III) Complexes. Journal of Physical Chemistry B, 2015, 119, 7378-7392.	2.6	11

#	Article	IF	Citations
91	Ultrafast excited state dynamics of [Cr(CO)₄(bpy)]: revealing the relaxation between triplet charge-transfer states. RSC Advances, 2016, 6, 20507-20515.	3.6	11
92	A Homoleptic Trisbidentate Ru(II) Complex of a Novel Bidentate Biheteroaromatic Ligand Based on Quinoline and Pyrazole Groups: Structural, Electrochemical, Photophysical, and Computational Characterization. Inorganic Chemistry, 2014, 53, 12778-12790.	4.0	10
93	Electro-mechanically switchable hydrocarbons based on [8]annulenes. Nature Communications, 2022, 13, 860.	12.8	10
94	Light-harvesting and electronic contacting capabilities of Ru(ii) Ipa rod and star complexesâ€“first principles predictions. RSC Advances, 2012, 2, 7868.	3.6	9
95	Diastereomerization Dynamics of a Bistridentate Ru^{II} Complex. Inorganic Chemistry, 2016, 55, 3015-3022.	4.0	8
96	Density Functional Theory Study of NO Adsorbed in A-Zeolite. Journal of Physical Chemistry B, 2005, 109, 7948-7951.	2.6	7
97	Excited State Dynamics of Bistridentate and Trisbidentate Ru^{II} Complexes of Quinoline-Pyrazole Ligands. Inorganic Chemistry, 2019, 58, 16354-16363.	4.0	7
98	Direct ESR evidence for SH2 type reaction of methyl radical with methylsilane and methylgermane in a low temperature solid: A deuterium labeling study. Chemical Physics Letters, 2005, 410, 1-5.	2.6	6
99	Material Dependence of Water Interactions with Metal Oxide Nanoparticles. Advances in Quantum Chemistry, 2014, 69, 303-332.	0.8	6
100	Chemical consequences of pyrazole orientation in Ru^{II} complexes of unsymmetric quinolineâ€“pyrazole ligands. Dalton Transactions, 2016, 45, 11723-11732.	3.3	6
101	HERFD-XANES probes of electronic structures of iron^{II/III} carbene complexes. Physical Chemistry Chemical Physics, 2020, 22, 9067-9073.	2.8	6
102	Design of robust 2,2â€²-bipyridine ligand linkers for the stable immobilization of molecular catalysts on silicon(111) surfaces. Physical Chemistry Chemical Physics, 2021, 23, 9921-9929.	2.8	6
103	Computational characterization of competing energy and electron transfer states in bimetallic donor-acceptor systems for photocatalytic conversion. Journal of Chemical Physics, 2016, 145, 104310.	3.0	5
104	Influence of Triplet Surface Properties on Excited-State Deactivation of Expanded Cage Bis(tridentate)Ruthenium(II) Complexes. Journal of Physical Chemistry A, 2019, 123, 5293-5299.	2.5	5
105	Spin propensity in resonant photoemission of transition metal complexes. Physical Review Research, 2021, 3, .	3.6	5
106	CHAPTER 3. Multiscale Modelling of Interfacial Electron Transfer. RSC Energy and Environment Series, 2013, , 77-110.	0.5	4
107	Quantum chemical calculations of the structural influence on electronic properties in TiO2 nanocrystals. Molecular Physics, 2017, 115, 2209-2217.	1.7	3
108	INDO calculations of small copper clusters and CO adsorbed on copper(100) surfaces. Journal of Computational Chemistry, 2000, 21, 1221-1228.	3.3	2

#	Article	IF	Citations
109	Quantum-chemical calculations of dye-sensitized semiconductor nanocrystals. , 2006, , .		2
110	Computational study of the catalytic effect of platinum on the decomposition of DNT. International Journal of Quantum Chemistry, 2012, 112, 1852-1858.	2.0	1
111	Inside Back Cover: A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3â€triazolâ€5â€ylidene) Ligands: Taming the MLCT Excited State of Iron(II) (Chem. Eur. J. 9/2015). Chemistry - A European Journal, 2015, 21, 3831-3831.	3.3	1
112	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. ChemSusChem, 2016, 9, 652-652.	6.8	1
113	Design, Synthesis and Computational Study of Fluorinated Quinoxalineâ€Oligothiopheneâ€based Conjugated Polymers with Broad Spectral Coverage. ChemPhysChem, 2018, 19, 3393-3400.	2.1	1
114	How Will the Emerging Plurality of Lives Change How We Conceive of and Relate to Life?. Challenges, 2019, 10, 32.	1.7	1
115	Resonant X-ray photo-oxidation of light-harvesting iron (II/III) N-heterocyclic carbene complexes. Scientific Reports, 2021, 11, 22144.	3.3	1
116	Photovoltaics and bio-inspired light harvesting: general discussion. Faraday Discussions, 2019, 216, 269-300.	3.2	0
117	Photo-induced electron transfer: general discussion. Faraday Discussions, 2019, 216, 434-459.	3.2	0