Petter Persson

List of Publications by Year
in descending order

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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	Electro-mechanically switchable hydrocarbons based on [8]annulenes. Nature Communications, 2022, 13, 860.	12.8	10
2	Photofunctionality of iron(III) N-heterocyclic carbenes and related d transition metal complexes. Coordination Chemistry Reviews, 2021, 426, 213517.	18.8	44
3	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
4	Spin propensity in resonant photoemission of transition metal complexes. Physical Review Research, 2021, 3, .	3.6	5
5	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
6	Resonant X-ray photo-oxidation of light-harvesting iron (II/III) N-heterocyclic carbene complexes. Scientific Reports, 2021, 11, 22144.	3.3	1
7	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
8	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
9	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
10	A Stable Homoleptic Organometallic Iron(IV) Complex. Chemistry - A European Journal, 2020, 26, 12728-12732.	3.3	21
11	Photophysics and Photochemistry of Iron Carbene Complexes for Solar Energy Conversion and Photocatalysis. Catalysts, 2020, 10, 315.	3.5	52
12	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. Nature Communications, 2020, 11, 634.	12.8	75
13	Site-Selective Orbital Interactions in an Ultrathin Iron-Carbene Photosensitizer Film. Journal of Physical Chemistry A, 2020, 124, 1603-1609.	2.5	12
14	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
15	HERFD-XANES probes of electronic structures of iron^{II/III} carbene complexes. Physical Chemistry Chemical Physics, 2020, 22, 9067-9073.	2.8	6
16	How Will the Emerging Plurality of Lives Change How We Conceive of and Relate to Life?. Challenges, 2019, 10, 32.	1.7	1
17	Photovoltaics and bio-inspired light harvesting: general discussion. Faraday Discussions, 2019, 216, 269-300.	3.2	0
18	Photo-induced electron transfer: general discussion. Faraday Discussions, 2019, 216, 434-459.	3.2	0

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19	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
20	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
21	Band-selective dynamics in charge-transfer excited iron carbene complexes. Faraday Discussions, 2019, 216, 191-210.	3.2	12
22	Excited State Dynamics of Bistridentate and Trisbidentate Ru^{II} Complexes of Quinoline-Pyrazole Ligands. Inorganic Chemistry, 2019, 58, 16354-16363.	4.0	7
23	Luminescence and reactivity of a charge-transfer excited iron complex with nanosecond lifetime. Science, 2019, 363, 249-253.	12.6	249
24	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
25	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
26	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
27	Design, Synthesis and Computational Study of Fluorinated Quinoxalineâ€Oligothiopheneâ€based Conjugated Polymers with Broad Spectral Coverage. ChemPhysChem, 2018, 19, 3393-3400.	2.1	1
28	Defining donor and acceptor strength in conjugated copolymers. Molecular Physics, 2017, 115, 485-496.	1.7	14
29	Quantum chemical calculations of the structural influence on electronic properties in TiO2 nanocrystals. Molecular Physics, 2017, 115, 2209-2217.	1.7	3
30	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
31	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
32	A low-spin Fe(iii) complex with 100-ps ligand-to-metal charge transfer photoluminescence. Nature, 2017, 543, 695-699.	27.8	287
33	Ultrafast Electron Dynamics in Solar Energy Conversion. Chemical Reviews, 2017, 117, 10940-11024.	47.7	266
34	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
35	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. ChemSusChem, 2016, 9, 667-675.	6.8	36
36	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. ChemSusChem, 2016, 9, 652-652.	6.8	1

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37	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
38	Fe N-Heterocyclic Carbene Complexes as Promising Photosensitizers. Accounts of Chemical Research, 2016, 49, 1477-1485.	15.6	197
39	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
40	Chemical consequences of pyrazole orientation in Ru^{II} complexes of unsymmetric quinolineâ€“pyrazole ligands. Dalton Transactions, 2016, 45, 11723-11732.	3.3	6
41	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
42	Diastereomerization Dynamics of a Bistridentate Ru^{II} Complex. Inorganic Chemistry, 2016, 55, 3015-3022.	4.0	8
43	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
44	Dâ€“A₁â€“Dâ€“A₂ Copolymers with Extended Donor Segments for Efficient Polymer Solar Cells. Macromolecules, 2015, 48, 1009-1016.	4.8	82
45	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
46	Temperature-Dependent Optical Properties of Flexible Donorâ€“Acceptor Polymers. Journal of Physical Chemistry C, 2015, 119, 6453-6463.	3.1	17
47	Rational design of Dâ€“A₁â€“Dâ€“A₂ conjugated polymers with superior spectral coverage. Physical Chemistry Chemical Physics, 2015, 17, 26677-26689.	2.8	12
48	Iron sensitizer converts light to electrons with 92% yield. Nature Chemistry, 2015, 7, 883-889.	13.6	193
49	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
50	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
51	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
52	Material Dependence of Water Interactions with Metal Oxide Nanoparticles. Advances in Quantum Chemistry, 2014, 69, 303-332.	0.8	6
53	Orbital Topology Controlling Charge Injection in Quantum-Dot-Sensitized Solar Cells. Journal of Physical Chemistry Letters, 2014, 5, 1157-1162.	4.6	27
54	Light-harvesting capabilities of low band gap donorâ€“acceptor polymers. Physical Chemistry Chemical Physics, 2014, 16, 24853-24865.	2.8	28

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55	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
56	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
57	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
58	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. Langmuir, 2013, 29, 7838-7846.	3.5	96
59	Conformation sensitive charge transport in conjugated polymers. Applied Physics Letters, 2013, 103, 213303.	3.3	11
60	CHAPTER 3. Multiscale Modelling of Interfacial Electron Transfer. RSC Energy and Environment Series, 2013, , 77-110.	0.5	4
61	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
62	Excited state potential energy surfaces of bistridentate RuII complexes â€“ A TD-DFT study. Chemical Physics, 2012, 407, 76-82.	1.9	29
63	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
64	Photoinduced electron transfer processes in dye-semiconductor systems with different spacer groups. Journal of Chemical Physics, 2012, 137, 22A529.	3.0	41
65	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
66	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
67	The electronic structure and reflectivity of PEDOT:PSS from density functional theory. Chemical Physics, 2011, 384, 44-51.	1.9	102
68	Meta-substituted RuII rigid rods for sensitization of TiO2. Journal of Photochemistry and Photobiology A: Chemistry, 2009, 206, 155-163.	3.9	12
69	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
70	Large Footprint Pyrene Chromophores Anchored to Planar and Colloidal Metal Oxide Thin Films. Langmuir, 2009, 25, 9219-9226.	3.5	21
71	Calculations of interfacial interactions in pyrene-Ipa rod sensitized nanostructured TiO2. Dalton Transactions, 2009, , 10021.	3.3	23
72	On the excited-state multi-dimensionality in cyanines. Chemical Physics Letters, 2008, 455, 13-19.	2.6	12

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73	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
74	Dynamical Simulation of Photoinduced Electron Transfer Reactions in Dyeâ^'Semiconductor Systems with Different Anchor Groups. Journal of Physical Chemistry C, 2008, 112, 12326-12333.	3.1	81
75	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
76	Steric Influence on the Excited-State Lifetimes of Ruthenium Complexes with Bipyridylâ^'Alkanyleneâ^'Pyridyl Ligands. Inorganic Chemistry, 2008, 47, 3540-3548.	4.0	127
77	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
78	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
79	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
80	Synthesis and Electron Transfer Studies of Rutheniumâ^'Terpyridine-Based Dyads Attached to Nanostructured TiO2. Inorganic Chemistry, 2007, 46, 638-651.	4.0	63
81	Cyclometallated Iridium and Platinum Complexes with Noninnocent Ligands. Inorganic Chemistry, 2007, 46, 3865-3875.	4.0	57
82	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
83	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
84	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
85	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
86	A 3.0 Î¼s Room Temperature Excited State Lifetime of a Bistridentate RuIIâ^'Polypyridine Complex for Rod-like Molecular Arrays. Journal of the American Chemical Society, 2006, 128, 12616-12617.	13.7	203
87	Photochemistry of Bromofluorobenzenes. Journal of Physical Chemistry A, 2006, 110, 7045-7056.	2.5	36
88	DFT study of bare and dye-sensitized TiO2 clusters and nanocrystals. International Journal of Quantum Chemistry, 2006, 106, 3214-3234.	2.0	230
89	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
90	Quantum-chemical calculations of dye-sensitized semiconductor nanocrystals. , 2006, , .		2

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91	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
92	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
93	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
94	Density Functional Theory Study of NO Adsorbed in A-Zeolite. Journal of Physical Chemistry B, 2005, 109, 7948-7951.	2.6	7
95	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
96	Photodissociation of bromobenzene, dibromobenzene, and 1,3,5-tribromobenzene. Journal of Chemical Physics, 2004, 120, 6502-6509.	3.0	44
97	Multireference calculations of the phosphorescence and photodissociation of chlorobenzene. Journal of Chemical Physics, 2004, 121, 11000.	3.0	27
98	Theoretical Study of the Fast Photodissociation Channels of the Monohalobenzenes. Journal of Physical Chemistry A, 2004, 108, 2339-2345.	2.5	59
99	Theoretical study of the photodissociation of low lying excited states of hydrogen peroxide. Molecular Physics, 2004, 102, 2575-2584.	1.7	11
100	Bi-isonicotinic acid on rutile (110): calculated molecular and electronic structure. Surface Science, 2003, 529, 47-58.	1.9	35
101	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
102	The Smallest Possible Nanocrystals of Semiionic Oxides. Journal of Physical Chemistry B, 2003, 107, 3336-3339.	2.6	68
103	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
104	Electron dynamics within Ru-2,2â€²-bipyridine complexesâ€”an N1s core level excitation study. Chemical Physics, 2002, 285, 167-176.	1.9	18
105	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
106	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. Nature, 2002, 418, 620-623.	27.8	346
107	Electronic interactions between aromatic adsorbates and metal oxide substrates calculated from first principles. Chemical Physics Letters, 2002, 364, 469-474.	2.6	60
108	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

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109	INDO calculations of small copper clusters and CO adsorbed on copper(100) surfaces. Journal of Computational Chemistry, 2000, 21, 1221-1228.	3.3	2
110	Binding of bi-isonicotinic acid to anatase TiO2 (101). Solar Energy Materials and Solar Cells, 2000, 63, 139-148.	6.2	50
111	Periodic Hartreeâ€“Fock study of the adsorption of formic acid on ZnO(1010). Chemical Physics Letters, 2000, 321, 302-308.	2.6	63
112	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
113	Quantum Chemical Study of Photoinjection Processes in Dye-Sensitized TiO2Nanoparticles. Journal of Physical Chemistry B, 2000, 104, 10348-10351.	2.6	333
114	XPS studies of Ru-polypyridine complexes for solar cell applications. Journal of Chemical Physics, 1999, 111, 2744-2750.	3.0	88
115	Adsorption of bi-isonicotinic acid on rutile TiO2(110). Journal of Chemical Physics, 1999, 110, 5913-5918.	3.0	165
116	Periodic INDO calculations of organic adsorbates on a TiO2 surface. International Journal of Quantum Chemistry, 1998, 70, 1055-1066.	2.0	51
117	Siteâ€selective participator decay of coreâ€excited butadiene. Journal of Chemical Physics, 1996, 105, 10719-10724.	3.0	15