

Petter Persson

List of Publications by Year in descending order

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117
papers

7,280
citations

44042

48
h-index

54882

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. <i>Nature</i> , 2002, 418, 620-623.	13.7	346
2	Quantum Chemical Study of Photoinjection Processes in Dye-Sensitized TiO ₂ Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2000, 104, 10348-10351.	1.2	333
3	A low-spin Fe(III) complex with 100-ps ligand-to-metal charge transfer photoluminescence. <i>Nature</i> , 2017, 543, 695-699.	13.7	287
4	Ultrafast Electron Dynamics in Solar Energy Conversion. <i>Chemical Reviews</i> , 2017, 117, 10940-11024.	23.0	266
5	Quantum Chemical Calculations of the Influence of Anchor-Cum-Spacer Groups on Femtosecond Electron Transfer Times in Dye-Sensitized Semiconductor Nanocrystals. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 441-451.	2.3	249
6	Luminescence and reactivity of a charge-transfer excited iron complex with nanosecond lifetime. <i>Science</i> , 2019, 363, 249-253.	6.0	249
7	DFT study of bare and dye-sensitized TiO ₂ clusters and nanocrystals. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 3214-3234.	1.0	230
8	A 3.0 ns Room Temperature Excited State Lifetime of a Bistridentate Ru(II)-Polypyridine Complex for Rod-like Molecular Arrays. <i>Journal of the American Chemical Society</i> , 2006, 128, 12616-12617.	6.6	203
9	Fe(II)-Heterocyclic Carbene Complexes as Promising Photosensitizers. <i>Accounts of Chemical Research</i> , 2016, 49, 1477-1485.	7.6	197
10	Iron sensitizer converts light to electrons with 92% yield. <i>Nature Chemistry</i> , 2015, 7, 883-889.	6.6	193
11	Calculated Structural and Electronic Interactions of the Ruthenium Dye N3 with a Titanium Dioxide Nanocrystal. <i>Journal of Physical Chemistry B</i> , 2005, 109, 11918-11924.	1.2	181
12	Bistridentate Ruthenium(II) polypyridyl-Type Complexes with Microsecond MLCT State Lifetimes: Sensitizers for Rod-Like Molecular Arrays. <i>Journal of the American Chemical Society</i> , 2008, 130, 15533-15542.	6.6	177
13	Adsorption of bi-isonicotinic acid on rutile TiO ₂ (110). <i>Journal of Chemical Physics</i> , 1999, 110, 5913-5918.	1.2	165
14	Phosphonic acid adsorption at the TiO ₂ anatase (101) surface investigated by periodic hybrid HF-DFT computations. <i>Surface Science</i> , 2005, 582, 49-60.	0.8	163
15	Fe(II)-Hexa(1,2,3-triazol-5-ylidene) Carbene Complex with a 528 ps Metal-to-Ligand Charge-Transfer Excited-State Lifetime. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 459-463.	2.1	151
16	Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14645-14654.	1.5	138
17	Anchor group influence on molecule-metal oxide interfaces: Periodic hybrid DFT study of pyridine bound to TiO ₂ via carboxylic and phosphonic acid. <i>Chemical Physics Letters</i> , 2005, 415, 375-380.	1.2	137
18	A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3-triazol-5-ylidene) Ligands: Taming the MLCT Excited State of Iron(II). <i>Chemistry - A European Journal</i> , 2015, 21, 3628-3639.	1.7	132

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19	Steric Influence on the Excited-State Lifetimes of Ruthenium Complexes with Bipyridyl-alkylene-pyridyl Ligands. <i>Inorganic Chemistry</i> , 2008, 47, 3540-3548.	1.9	127
20	Exceptional Excited-State Lifetime of an Iron(II)-N-Heterocyclic Carbene Complex Explained. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2066-2071.	2.1	125
21	Spacer and Anchor Effects on the Electronic Coupling in Ruthenium-bis-Terpyridine Dye-Sensitized TiO ₂ Nanocrystals Studied by DFT. <i>Journal of Physical Chemistry B</i> , 2006, 110, 20513-20525.	1.2	115
22	PES Studies of Ru(dcbpy) ₂ (NCS) ₂ Adsorption on Nanostructured ZnO for Solar Cell Applications. <i>Journal of Physical Chemistry B</i> , 2002, 106, 10102-10107.	1.2	106
23	The electronic structure and reflectivity of PEDOT:PSS from density functional theory. <i>Chemical Physics</i> , 2011, 384, 44-51.	0.9	102
24	Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution. <i>Chemical Science</i> , 2017, 8, 515-523.	3.7	102
25	Development of the ReaxFF reactive force field for mechanistic studies of catalytic selective oxidation processes on BiMoO _x . <i>Topics in Catalysis</i> , 2006, 38, 93.	1.3	98
26	Development of a ReaxFF Reactive Force Field for Titanium Dioxide/Water Systems. <i>Langmuir</i> , 2013, 29, 7838-7846.	1.6	96
27	Finding intersections between electronic excited state potential energy surfaces with simultaneous ultrafast X-ray scattering and spectroscopy. <i>Chemical Science</i> , 2019, 10, 5749-5760.	3.7	90
28	XPS studies of Ru-polypyridine complexes for solar cell applications. <i>Journal of Chemical Physics</i> , 1999, 111, 2744-2750.	1.2	88
29	Dye-Sensitization of the TiO ₂ Rutile (110) Surface by Perylene Dyes: Quantum-Chemical Periodic B3LYP Computations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 12116-12123.	1.5	84
30	Influence of Triplet State Multidimensionality on Excited State Lifetimes of Bis-tridentate Ru(II) Complexes: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1041-1050.	1.1	84
31	PAA ₁ -PAA ₂ Copolymers with Extended Donor Segments for Efficient Polymer Solar Cells. <i>Macromolecules</i> , 2015, 48, 1009-1016.	2.2	82
32	Dynamical Simulation of Photoinduced Electron Transfer Reactions in Dye-Semiconductor Systems with Different Anchor Groups. <i>Journal of Physical Chemistry C</i> , 2008, 112, 12326-12333.	1.5	81
33	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. <i>Nature Communications</i> , 2020, 11, 634.	5.8	75
34	N _K x-ray absorption study of the bonding interaction of bi-isonicotinic acid adsorbed on rutile TiO ₂ (110). <i>Journal of Chemical Physics</i> , 2000, 112, 3945-3948.	1.2	68
35	The Smallest Possible Nanocrystals of Semiionic Oxides. <i>Journal of Physical Chemistry B</i> , 2003, 107, 3336-3339.	1.2	68
36	Periodic Hartree-Fock study of the adsorption of formic acid on ZnO(1010). <i>Chemical Physics Letters</i> , 2000, 321, 302-308.	1.2	63

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37	Synthesis and Electron Transfer Studies of Ruthenium ^{II} -Terpyridine-Based Dyads Attached to Nanostructured TiO ₂ . <i>Inorganic Chemistry</i> , 2007, 46, 638-651.	1.9	63
38	Electronic interactions between aromatic adsorbates and metal oxide substrates calculated from first principles. <i>Chemical Physics Letters</i> , 2002, 364, 469-474.	1.2	60
39	Theoretical Study of the Fast Photodissociation Channels of the Monohalobenzenes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2339-2345.	1.1	59
40	Computational Study of the Lowest Triplet State of Ruthenium Polypyridyl Complexes Used in Artificial Photosynthesis. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4470-4476.	1.1	58
41	Cyclometallated Iridium and Platinum Complexes with Noninnocent Ligands. <i>Inorganic Chemistry</i> , 2007, 46, 3865-3875.	1.9	57
42	Structural study of adsorption of isonicotinic acid and related molecules on rutile TiO ₂ (110) I: XAS and STM. <i>Surface Science</i> , 2003, 540, 39-54.	0.8	52
43	Solvent control of charge transfer excited state relaxation pathways in [Fe(2,2'-bipyridine) ₄ (CN) ₄] ²⁺ . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4238-4249.	1.3	52
44	Photophysics and Photochemistry of Iron Carbene Complexes for Solar Energy Conversion and Photocatalysis. <i>Catalysts</i> , 2020, 10, 315.	1.6	52
45	Periodic INDO calculations of organic adsorbates on a TiO ₂ surface. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 1055-1066.	1.0	51
46	Binding of bi-isonicotinic acid to anatase TiO ₂ (101). <i>Solar Energy Materials and Solar Cells</i> , 2000, 63, 139-148.	3.0	50
47	Microsecond Photoluminescence and Photoreactivity of a Metal-Centered Excited State in a Hexacarbene ⁺ Co(III) Complex. <i>Journal of the American Chemical Society</i> , 2021, 143, 1307-1312.	6.6	50
48	Tracking the picosecond deactivation dynamics of a photoexcited iron carbene complex by time-resolved X-ray scattering. <i>Chemical Science</i> , 2018, 9, 405-414.	3.7	49
49	Photodissociation of bromobenzene, dibromobenzene, and 1,3,5-tribromobenzene. <i>Journal of Chemical Physics</i> , 2004, 120, 6502-6509.	1.2	44
50	Photofunctionality of iron(III) N-heterocyclic carbenes and related d transition metal complexes. <i>Coordination Chemistry Reviews</i> , 2021, 426, 213517.	9.5	44
51	Quantum chemical prediction of the adsorption conformations and dynamics at HCOOH-covered ZnO(1010) surfaces. <i>International Journal of Quantum Chemistry</i> , 2002, 89, 172-180.	1.0	41
52	Photoinduced electron transfer processes in dye-semiconductor systems with different spacer groups. <i>Journal of Chemical Physics</i> , 2012, 137, 22A529.	1.2	41
53	Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2'-bipyridine) ₂ (CN) ₂]. <i>Structural Dynamics</i> , 2017, 4, 044030.	0.9	41
54	Hot Branching Dynamics in a Light ⁺ Harvesting Iron Carbene Complex Revealed by Ultrafast X-ray Emission Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 364-372.	7.2	41

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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. <i>Inorganic Chemistry</i> , 2013, 52, 5128-5137.	1.9	40
56	Photochemistry of Bromofluorobenzenes. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7045-7056.	1.1	36
57	Shake-up and shake-off excitations with associated electron losses in X-ray studies of proteins. <i>Protein Science</i> , 2009, 10, 2480-2484.	3.1	36
58	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. <i>ChemSusChem</i> , 2016, 9, 667-675.	3.6	36
59	Bi-isonicotinic acid on rutile (110): calculated molecular and electronic structure. <i>Surface Science</i> , 2003, 529, 47-58.	0.8	35
60	Tracing the Full Bimolecular Photocycle of Iron(III)-Carbene Light Harvesters in Electron-Donating Solvents. <i>Journal of the American Chemical Society</i> , 2020, 142, 8565-8569.	6.6	34
61	High-Performance Hole Transport and Quasi-Balanced Ambipolar OFETs Based on Thieno-benzothioindigo Polymers. <i>Advanced Electronic Materials</i> , 2016, 2, 1500313.	2.6	32
62	Calculated Optoelectronic Properties of Ruthenium Tris-bipyridine Dyes Containing Oligophenyleneethynylene Rigid Rod Linkers in Different Chemical Environments. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1487-1497.	1.1	30
63	Excited state potential energy surfaces of bistridentate Rull complexes - A TD-DFT study. <i>Chemical Physics</i> , 2012, 407, 76-82.	0.9	29
64	Emerging polymorphism in nanostructured TiO ₂ : Quantum chemical comparison of anatase, rutile, and brookite clusters. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2611-2620.	1.0	29
65	Light-harvesting capabilities of low band gap donor-acceptor polymers. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24853-24865.	1.3	28
66	Multireference calculations of the phosphorescence and photodissociation of chlorobenzene. <i>Journal of Chemical Physics</i> , 2004, 121, 11000.	1.2	27
67	Frequency dispersed transient absorption spectra of dissolved perylene: A case study using the density matrix version of the MCTDH method. <i>Chemical Physics</i> , 2008, 347, 152-165.	0.9	27
68	Orbital Topology Controlling Charge Injection in Quantum-Dot-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1157-1162.	2.1	27
69	One-Step Synthesis of Precursor Oligomers for Organic Photovoltaics: A Comparative Study between Polymers and Small Molecules. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 27106-27114.	4.0	25
70	Calculations of interfacial interactions in pyrene- <i>lpa</i> rod sensitized nanostructured TiO ₂ . <i>Dalton Transactions</i> , 2009, , 10021.	1.6	23
71	Quantum Chemical Calculations of Side-Group Stacking and Electronic Properties in Thiophene-Quinoxaline Polymers. <i>Journal of Physical Chemistry C</i> , 2012, 116, 26700-26706.	1.5	23
72	Large Footprint Pyrene Chromophores Anchored to Planar and Colloidal Metal Oxide Thin Films. <i>Langmuir</i> , 2009, 25, 9219-9226.	1.6	21

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73	A Stable Homoleptic Organometallic Iron(IV) Complex. <i>Chemistry - A European Journal</i> , 2020, 26, 12728-12732.	1.7	21
74	Electron dynamics within Ru-2,2'-bipyridine complexes—an N1s core level excitation study. <i>Chemical Physics</i> , 2002, 285, 167-176.	0.9	18
75	Structures of Tetrafluorocyclopropene, Hexafluorocyclobutene, Octafluorocyclopentene and Related Perfluoroalkene Radical Anions Revealed by Electron Spin Resonance Spectroscopic and Computational Studies. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6307-6323.	1.1	18
76	Temperature-Dependent Optical Properties of Flexible Donor-Acceptor Polymers. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6453-6463.	1.5	17
77	Dye-sensitized solar cells based on Fe N-heterocyclic carbene photosensitizers with improved rod-like push-pull functionality. <i>Chemical Science</i> , 2021, 12, 16035-16053.	3.7	17
78	Site-selective participator decay of core-excited butadiene. <i>Journal of Chemical Physics</i> , 1996, 105, 10719-10724.	1.2	15
79	Triarylamine on Nanocrystalline TiO ₂ Studied in Its Reduced and Oxidized State by Photoelectron Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7182-7187.	1.2	14
80	Defining donor and acceptor strength in conjugated copolymers. <i>Molecular Physics</i> , 2017, 115, 485-496.	0.8	14
81	Electronic structure and excited state properties of iron carbene photosensitizers – A combined X-ray absorption and quantum chemical investigation. <i>Chemical Physics Letters</i> , 2017, 683, 559-566.	1.2	14
82	Hot Branching Dynamics in a Light-Harvesting Iron Carbene Complex Revealed by Ultrafast X-ray Emission Spectroscopy. <i>Angewandte Chemie</i> , 2020, 132, 372-380.	1.6	14
83	On the excited-state multi-dimensionality in cyanines. <i>Chemical Physics Letters</i> , 2008, 455, 13-19.	1.2	12
84	Meta-substituted Rull rigid rods for sensitization of TiO ₂ . <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2009, 206, 155-163.	2.0	12
85	Rational design of D ¹ -D ² conjugated polymers with superior spectral coverage. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26677-26689.	1.3	12
86	Band-selective dynamics in charge-transfer excited iron carbene complexes. <i>Faraday Discussions</i> , 2019, 216, 191-210.	1.6	12
87	Site-Selective Orbital Interactions in an Ultrathin Iron-Carbene Photosensitizer Film. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1603-1609.	1.1	12
88	Theoretical study of the photodissociation of low lying excited states of hydrogen peroxide. <i>Molecular Physics</i> , 2004, 102, 2575-2584.	0.8	11
89	Conformation sensitive charge transport in conjugated polymers. <i>Applied Physics Letters</i> , 2013, 103, 213303.	1.5	11
90	Exploring Photoinduced Excited State Evolution in Heterobimetallic Ru(II)-Co(III) Complexes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 7378-7392.	1.2	11

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91	Ultrafast excited state dynamics of $[\text{Cr}(\text{CO})_4(\text{bpy})]$: revealing the relaxation between triplet charge-transfer states. <i>RSC Advances</i> , 2016, 6, 20507-20515.	1.7	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. <i>Inorganic Chemistry</i> , 2014, 53, 12778-12790.	1.9	10
93	Electro-mechanically switchable hydrocarbons based on [8]annulenes. <i>Nature Communications</i> , 2022, 13, 860.	5.8	10
94	Light-harvesting and electronic contacting capabilities of Ru(II) Ipa rod and star complexes—first principles predictions. <i>RSC Advances</i> , 2012, 2, 7868.	1.7	9
95	Diastereomerization Dynamics of a Bistridentate Ru ^{II} Complex. <i>Inorganic Chemistry</i> , 2016, 55, 3015-3022.	1.9	8
96	Density Functional Theory Study of NO Adsorbed in A-Zeolite. <i>Journal of Physical Chemistry B</i> , 2005, 109, 7948-7951.	1.2	7
97	Excited State Dynamics of Bistridentate and Trisbidentate Ru ^{II} Complexes of Quinoline-Pyrazole Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 16354-16363.	1.9	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. <i>Chemical Physics Letters</i> , 2005, 410, 1-5.	1.2	6
99	Material Dependence of Water Interactions with Metal Oxide Nanoparticles. <i>Advances in Quantum Chemistry</i> , 2014, 69, 303-332.	0.4	6
100	Chemical consequences of pyrazole orientation in Ru ^{II} complexes of unsymmetric quinoline—pyrazole ligands. <i>Dalton Transactions</i> , 2016, 45, 11723-11732.	1.6	6
101	HERFD-XANES probes of electronic structures of iron ^{II/III} carbene complexes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9067-9073.	1.3	6
102	Design of robust 2,2'-bipyridine ligand linkers for the stable immobilization of molecular catalysts on silicon(111) surfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 9921-9929.	1.3	6
103	Computational characterization of competing energy and electron transfer states in bimetallic donor-acceptor systems for photocatalytic conversion. <i>Journal of Chemical Physics</i> , 2016, 145, 104310.	1.2	5
104	Influence of Triplet Surface Properties on Excited-State Deactivation of Expanded Cage Bis(tridentate)Ruthenium(II) Complexes. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5293-5299.	1.1	5
105	Spin propensity in resonant photoemission of transition metal complexes. <i>Physical Review Research</i> , 2021, 3, .	1.3	5
106	CHAPTER 3. Multiscale Modelling of Interfacial Electron Transfer. <i>RSC Energy and Environment Series</i> , 2013, , 77-110.	0.2	4
107	Quantum chemical calculations of the structural influence on electronic properties in TiO ₂ nanocrystals. <i>Molecular Physics</i> , 2017, 115, 2209-2217.	0.8	3
108	INDO calculations of small copper clusters and CO adsorbed on copper(100) surfaces. <i>Journal of Computational Chemistry</i> , 2000, 21, 1221-1228.	1.5	2

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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.	1.0	1
111	Inside Back Cover: A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3-triazol-5-ylidene) Ligands: Taming the MLCT Excited State of Iron(II) (Chem. Eur. J. 9/2015). Chemistry - A European Journal, 2015, 21, 3831-3831.	1.7	1
112	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. ChemSusChem, 2016, 9, 652-652.	3.6	1
113	Design, Synthesis and Computational Study of Fluorinated Quinoxaline-Oligothiophene-based Conjugated Polymers with Broad Spectral Coverage. ChemPhysChem, 2018, 19, 3393-3400.	1.0	1
114	How Will the Emerging Plurality of Lives Change How We Conceive of and Relate to Life?. Challenges, 2019, 10, 32.	0.9	1
115	Resonant X-ray photo-oxidation of light-harvesting iron (II/III) N-heterocyclic carbene complexes. Scientific Reports, 2021, 11, 22144.	1.6	1
116	Photovoltaics and bio-inspired light harvesting: general discussion. Faraday Discussions, 2019, 216, 269-300.	1.6	0
117	Photo-induced electron transfer: general discussion. Faraday Discussions, 2019, 216, 434-459.	1.6	0