Petter Persson

List of Publications by Citations

115 papers	6,188 citations	43 h-index	77 g-index
120 ext. papers	6,726 ext. citations	6.6 avg, IF	5.59 L-index

#	Paper	IF	Citations
115	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. *Nature*, **2002**, 418, 620-3	50.4	321
114	Quantum Chemical Study of Photoinjection Processes in Dye-Sensitized TiO2 Nanoparticles. *Journal of Physical Chemistry B*, **2000**, 104, 10348-10351	3.4	309
113	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, 441-51	6.4	238
112	DFT study of bare and dye-sensitized TiO2 clusters and nanocrystals. *International Journal of Quantum Chemistry*, **2006**, 106, 3214-3234	2.1	212
111	A low-spin Fe(iii) complex with 100-ps ligand-to-metal charge transfer photoluminescence. *Nature*, **2017**, 543, 695-699	50.4	205
110	Ultrafast Electron Dynamics in Solar Energy Conversion. *Chemical Reviews*, **2017**, 117, 10940-11024	68.1	202
109	Calculated structural and electronic interactions of the ruthenium dye N3 with a titanium dioxide nanocrystal. *Journal of Physical Chemistry B*, **2005**, 109, 11918-24	3.4	175
108	A 3.0 micros room temperature excited state lifetime of a bistridentate RuII-polypyridine complex for rod-like molecular arrays. *Journal of the American Chemical Society*, **2006**, 128, 12616-7	16.4	174
107	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, 15533-42	16.4	162
106	Iron sensitizer converts light to electrons with 92% yield. *Nature Chemistry*, **2015**, 7, 883-9	17.6	161
105	Adsorption of bi-isonicotinic acid on rutile TiO2(110). *Journal of Chemical Physics*, **1999**, 110, 5913-5918	3.9	159
104	Phosphonic acid adsorption at the TiO2 anatase (101) surface investigated by periodic hybrid HF-DFT computations. *Surface Science*, **2005**, 582, 49-60	1.8	156
103	Luminescence and reactivity of a charge-transfer excited iron complex with nanosecond lifetime. *Science*, **2019**, 363, 249-253	33.3	155
102	Fe N-Heterocyclic Carbene Complexes as Promising Photosensitizers. *Accounts of Chemical Research*, **2016**, 49, 1477-85	24.3	148
101	Anchor group influence on molecule–metal oxide interfaces: Periodic hybrid DFT study of pyridine bound to TiO2 via carboxylic and phosphonic acid. *Chemical Physics Letters*, **2005**, 415, 375-380	2.5	130
100	Steric influence on the excited-state lifetimes of ruthenium complexes with bipyridyl-alkanylene-pyridyl ligands. *Inorganic Chemistry*, **2008**, 47, 3540-8	5.1	112
99	Spacer and anchor effects on the electronic coupling in ruthenium-bis-terpyridine dye-sensitized TiO2 nanocrystals studied by DFT. *Journal of Physical Chemistry B*, **2006**, 110, 20513-25	3.4	112

98	Exceptional Excited-State Lifetime of an Iron(II)-N-Heterocyclic Carbene Complex Explained. *Journal of Physical Chemistry Letters*, **2014**, 5, 2066-71	6.4	110
97	A heteroleptic ferrous complex with mesoionic bis(1,2,3-triazol-5-ylidene) ligands: taming the MLCT excited state of iron(II). *Chemistry - A European Journal*, **2015**, 21, 3628-39	4.8	106
96	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	3.8	106
95	Fe 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	6.4	101
94	PES Studies of Ru(dcbpyH2)2(NCS)2 Adsorption on Nanostructured ZnO for Solar Cell Applications. *Journal of Physical Chemistry B*, **2002**, 106, 10102-10107	3.4	101
93	Development of the ReaxFF reactive force field for mechanistic studies of catalytic selective oxidation processes on BiMoO x. *Topics in Catalysis*, **2006**, 38, 93	2.3	89
92	Dye-Sensitization of the TiO2 Rutile (110) Surface by Perylene Dyes: Quantum-Chemical Periodic B3LYP Computations. *Journal of Physical Chemistry C*, **2007**, 111, 12116-12123	3.8	82
91	XPS studies of Ru-polypyridine complexes for solar cell applications. *Journal of Chemical Physics*, **1999**, 111, 2744-2750	3.9	82
90	The electronic structure and reflectivity of PEDOT:PSS from density functional theory. *Chemical Physics*, **2011**, 384, 44-51	2.3	80
89	Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution. *Chemical Science*, **2017**, 8, 515-523	9.4	79
88	D–A1–D–A2 Copolymers with Extended Donor Segments for Efficient Polymer Solar Cells. *Macromolecules*, **2015**, 48, 1009-1016	5.5	78
87	Development of a ReaxFF reactive force field for titanium dioxide/water systems. *Langmuir*, **2013**, 29, 7838-46	4	77
86	Dynamical Simulation of Photoinduced Electron Transfer Reactions in Dye–Semiconductor Systems with Different Anchor Groups. *Journal of Physical Chemistry C*, **2008**, 112, 12326-12333	3.8	77
85	Influence of triplet state multidimensionality on excited state lifetimes of bis-tridentate RuII complexes: a computational study. *Journal of Physical Chemistry A*, **2012**, 116, 1041-50	2.8	75
84	N 1s 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	3.9	66
83	The Smallest Possible Nanocrystals of Semiionic Oxides. *Journal of Physical Chemistry B*, **2003**, 107, 3336-3339	3.4	63
82	Synthesis and electron transfer studies of ruthenium-terpyridine-based dyads attached to nanostructured TiO2. *Inorganic Chemistry*, **2007**, 46, 638-51	5.1	60
81	Periodic Hartree–Fock study of the adsorption of formic acid on ZnO(1010). *Chemical Physics Letters*, **2000**, 321, 302-308	2.5	60

80	Electronic interactions between aromatic adsorbates and metal oxide substrates calculated from first principles. *Chemical Physics Letters*, **2002**, 364, 469-474	2.5	58
79	Computational study of the lowest triplet state of ruthenium polypyridyl complexes used in artificial photosynthesis. *Journal of Physical Chemistry A*, **2008**, 112, 4470-6	2.8	56
78	Cyclometallated iridium and platinum complexes with noninnocent ligands. *Inorganic Chemistry*, **2007**, 46, 3865-75	5.1	55
77	Finding intersections between electronic excited state potential energy surfaces with simultaneous ultrafast X-ray scattering and spectroscopy. *Chemical Science*, **2019**, 10, 5749-5760	9.4	54
76	Theoretical Study of the Fast Photodissociation Channels of the Monohalobenzenes. *Journal of Physical Chemistry A*, **2004**, 108, 2339-2345	2.8	52
75	Structural study of adsorption of isonicotinic acid and related molecules on rutile TiO2(110) I: XAS and STM. *Surface Science*, **2003**, 540, 39-54	1.8	50
74	Binding of bi-isonicotinic acid to anatase TiO2 (1 0 1). *Solar Energy Materials and Solar Cells*, **2000**, 63, 139-148	6.4	49
73	Periodic INDO calculations of organic adsorbates on a TiO2 surface. *International Journal of Quantum Chemistry*, **1998**, 70, 1055-1066	2.1	47
72	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. *Nature Communications*, **2020**, 11, 634	17.4	41
71	Solvent control of charge transfer excited state relaxation pathways in [Fe(2,2′bipyridine)(CN)]. *Physical Chemistry Chemical Physics*, **2018**, 20, 4238-4249	3.6	41
70	Quantum chemical prediction of the adsorption conformations and dynamics at HCOOH-covered ZnO(1010) surfaces. *International Journal of Quantum Chemistry*, **2002**, 89, 172-180	2.1	41
69	Photodissociation of bromobenzene, dibromobenzene, and 1,3,5-tribromobenzene. *Journal of Chemical Physics*, **2004**, 120, 6502-9	3.9	40
68	Photoinduced electron transfer processes in dye-semiconductor systems with different spacer groups. *Journal of Chemical Physics*, **2012**, 137, 22A529	3.9	39
67	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, 5128-37	5.1	39
66	Ligand manipulation of charge transfer excited state relaxation and spin crossover in [Fe(2,2′bipyridine)(CN)]. *Structural Dynamics*, **2017**, 4, 044030	3.2	38
65	Tracking the picosecond deactivation dynamics of a photoexcited iron carbene complex by time-resolved X-ray scattering. *Chemical Science*, **2018**, 9, 405-414	9.4	35
64	Bi-isonicotinic acid on rutile (110): calculated molecular and electronic structure. *Surface Science*, **2003**, 529, 47-58	1.8	35
63	Photochemistry of bromofluorobenzenes. *Journal of Physical Chemistry A*, **2006**, 110, 7045-56	2.8	33

62	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. *ChemSusChem*, **2016**, 9, 667-75	8.3	31
61	High-Performance Hole Transport and Quasi-Balanced Ambipolar OFETs Based on D-A Thieno-benzo-isoindigo Polymers. *Advanced Electronic Materials*, **2016**, 2, 1500313	6.4	29
60	Shake-up and shake-off excitations with associated electron losses in X-ray studies of proteins. *Protein Science*, **2001**, 10, 2480-4	6.3	29
59	Calculated optoelectronic properties of ruthenium tris-bipyridine dyes containing oligophenyleneethynylene rigid rod linkers in different chemical environments. *Journal of Physical Chemistry A*, **2007**, 111, 1487-97	2.8	29
58	Photophysics and Photochemistry of Iron Carbene Complexes for Solar Energy Conversion and Photocatalysis. *Catalysts*, **2020**, 10, 315	4	28
57	Excited state potential energy surfaces of bistridentate RuII complexes - A TD-DFT study. *Chemical Physics*, **2012**, 407, 76-82	2.3	28
56	Hot Branching Dynamics in a Light-Harvesting Iron Carbene Complex Revealed by Ultrafast X-ray Emission Spectroscopy. *Angewandte Chemie - International Edition*, **2020**, 59, 364-372	16.4	28
55	Emerging polymorphism in nanostructured TiO2: Quantum chemical comparison of anatase, rutile, and brookite clusters. *International Journal of Quantum Chemistry*, **2013**, 113, 2611-2620	2.1	26
54	Orbital Topology Controlling Charge Injection in Quantum-Dot-Sensitized Solar Cells. *Journal of Physical Chemistry Letters*, **2014**, 5, 1157-62	6.4	25
53	Light-harvesting capabilities of low band gap donor-acceptor polymers. *Physical Chemistry Chemical Physics*, **2014**, 16, 24853-65	3.6	24
52	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	2.3	24
51	Multireference calculations of the phosphorescence and photodissociation of chlorobenzene. *Journal of Chemical Physics*, **2004**, 121, 11000-6	3.9	24
50	One-Step Synthesis of Precursor Oligomers for Organic Photovoltaics: A Comparative Study between Polymers and Small Molecules. *ACS Applied Materials & Interfaces*, **2015**, 7, 27106-14	9.5	23
49	Quantum Chemical Calculations of Side-Group Stacking and Electronic Properties in Thiophene-Quinoxaline Polymers. *Journal of Physical Chemistry C*, **2012**, 116, 26700-26706	3.8	22
48	Large footprint pyrene chromophores anchored to planar and colloidal metal oxide thin films. *Langmuir*, **2009**, 25, 9219-26	4	21
47	Calculations of interfacial interactions in pyrene-Ipa rod sensitized nanostructured TiO2. *Dalton Transactions*, **2009**, 10021-31	4.3	21
46	Microsecond Photoluminescence and Photoreactivity of a Metal-Centered Excited State in a Hexacarbene-Co(III) Complex. *Journal of the American Chemical Society*, **2021**, 143, 1307-1312	16.4	21
45	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, 6307-23	2.8	18

44	Photofunctionality of iron(III) N-heterocyclic carbenes and related d transition metal complexes. *Coordination Chemistry Reviews*, **2021**, 426, 213517	23.2	18
43	Electron dynamics within Ru-2,2?-bipyridine complexes□n N1s core level excitation study. *Chemical Physics*, **2002**, 285, 167-176	2.3	17
42	Temperature-Dependent Optical Properties of Flexible Donor□Acceptor Polymers. *Journal of Physical Chemistry C*, **2015**, 119, 6453-6463	3.8	16
41	Tracing the Full Bimolecular Photocycle of Iron(III)-Carbene Light Harvesters in Electron-Donating Solvents. *Journal of the American Chemical Society*, **2020**, 142, 8565-8569	16.4	15
40	Defining donor and acceptor strength in conjugated copolymers. *Molecular Physics*, **2017**, 115, 485-496	1.7	12
39	Electronic structure and excited state properties of iron carbene photosensitizers □A combined X-ray absorption and quantum chemical investigation. *Chemical Physics Letters*, **2017**, 683, 559-566	2.5	12
38	Rational design of D-A1-D-A2 conjugated polymers with superior spectral coverage. *Physical Chemistry Chemical Physics*, **2015**, 17, 26677-89	3.6	12
37	Triarylamine on Nanocrystalline TiO2 Studied in Its Reduced and Oxidized State by Photoelectron Spectroscopy. *Journal of Physical Chemistry B*, **2001**, 105, 7182-7187	3.4	12
36	Site-selective participator decay of core-excited butadiene. *Journal of Chemical Physics*, **1996**, 105, 10719-10724	3.1	12
35	Hot Branching Dynamics in a Light-Harvesting Iron Carbene Complex Revealed by Ultrafast X-ray Emission Spectroscopy. *Angewandte Chemie*, **2020**, 132, 372-380	3.6	12
34	Conformation sensitive charge transport in conjugated polymers. *Applied Physics Letters*, **2013**, 103, 213303	3.4	11
33	On the excited-state multi-dimensionality in cyanines. *Chemical Physics Letters*, **2008**, 455, 13-19	2.5	11
32	Theoretical study of the photodissociation of low lying excited states of hydrogen peroxide. *Molecular Physics*, **2004**, 102, 2575-2584	1.7	11
31	Band-selective dynamics in charge-transfer excited iron carbene complexes. *Faraday Discussions*, **2019**, 216, 191-210	3.6	9
30	Exploring Photoinduced Excited State Evolution in Heterobimetallic Ru(II)-Co(III) Complexes. *Journal of Physical Chemistry B*, **2015**, 119, 7378-92	3.4	9
29	Ultrafast excited state dynamics of [Cr(CO)4(bpy)]: revealing the relaxation between triplet charge-transfer states. *RSC Advances*, **2016**, 6, 20507-20515	3.7	9
28	Light-harvesting and electronic contacting capabilities of Ru(II) Ipa rod and star complexes□irst principles predictions. *RSC Advances*, **2012**, 2, 7868	3.7	9
27	Meta-substituted RuII rigid rods for sensitization of TiO2. *Journal of Photochemistry and Photobiology A: Chemistry*, **2009**, 206, 155-163	4.7	9

26	A Stable Homoleptic Organometallic Iron(IV) Complex. *Chemistry - A European Journal*, **2020**, 26, 12728-12732	4.8	8
25	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, 12778-90	5.1	8
24	Site-Selective Orbital Interactions in an Ultrathin Iron-Carbene Photosensitizer Film. *Journal of Physical Chemistry A*, **2020**, 124, 1603-1609	2.8	7
23	Diastereomerization Dynamics of a Bistridentate Ru(II) Complex. *Inorganic Chemistry*, **2016**, 55, 3015-22	5.1	7
22	Density functional theory study of NO adsorbed in A-zeolite. *Journal of Physical Chemistry B*, **2005**, 109, 7948-51	3.4	7
21	Chemical consequences of pyrazole orientation in Ru(II) complexes of unsymmetric quinoline-pyrazole ligands. *Dalton Transactions*, **2016**, 45, 11723-32	4.3	5
20	Material Dependence of Water Interactions with Metal Oxide Nanoparticles. *Advances in Quantum Chemistry*, **2014**, 69, 303-332	1.4	5
19	Excited State Dynamics of Bistridentate and Trisbidentate Ru Complexes of Quinoline-Pyrazole Ligands. *Inorganic Chemistry*, **2019**, 58, 16354-16363	5.1	5
18	HERFD-XANES probes of electronic structures of iron carbene complexes. *Physical Chemistry Chemical Physics*, **2020**, 22, 9067-9073	3.6	5
17	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	2.5	4
16	CHAPTER 3:Multiscale Modelling of Interfacial Electron Transfer. *RSC Energy and Environment Series* , **2013**, 77-110	0.6	4
15	Computational characterization of competing energy and electron transfer states in bimetallic donor-acceptor systems for photocatalytic conversion. *Journal of Chemical Physics*, **2016**, 145, 104310	3.9	4
14	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	2.8	3
13	Dye-sensitized solar cells based on Fe N-heterocyclic carbene photosensitizers with improved rod-like push-pull functionality.. *Chemical Science*, **2021**, 12, 16035-16053	9.4	3
12	Spin propensity in resonant photoemission of transition metal complexes. *Physical Review Research* , **2021**, 3,	3.9	3
11	Quantum chemical calculations of the structural influence on electronic properties in TiO2 nanocrystals. *Molecular Physics*, **2017**, 115, 2209-2217	1.7	2
10	INDO calculations of small copper clusters and CO adsorbed on copper(100) surfaces. *Journal of Computational Chemistry*, **2000**, 21, 1221-1228	3.5	2
9	Electro-mechanically switchable hydrocarbons based on [8]annulenes.. *Nature Communications*, **2022**, 13, 860	17.4	2

8	Water-Soluble Molecularly Imprinted Nanoparticles (MINPs) with Tailored, Functionalized, Modifiable Binding Pockets. *Chemistry - A European Journal*, **2014**, 21, 3831	4.8	1
7	Computational study of the catalytic effect of platinum on the decomposition of DNT. *International Journal of Quantum Chemistry*, **2012**, 112, 1852-1858	2.1	1
6	Resonant X-ray photo-oxidation of light-harvesting iron (II/III) N-heterocyclic carbene complexes. *Scientific Reports*, **2021**, 11, 22144	4.9	1
5	Molecular and Interfacial Calculations of Iron(II) Light Harvesters. *ChemSusChem*, **2016**, 9, 652-652	8.3	1
4	Design of robust 2,2′-bipyridine ligand linkers for the stable immobilization of molecular catalysts on silicon(111) surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 9921-9929	3.6	1
3	How Will the Emerging Plurality of Lives Change How We Conceive of and Relate to Life?. *Challenges*, **2019**, 10, 32	3.4	0
2	Photovoltaics and bio-inspired light harvesting: general discussion. *Faraday Discussions*, **2019**, 216, 269-300	3.6	
1	Design, Synthesis and Computational Study of Fluorinated Quinoxaline-Oligothiophene-based Conjugated Polymers with Broad Spectral Coverage. *ChemPhysChem*, **2018**, 19, 3393-3400	3.2	