Thomas Renger

List of Publications by Year
in descending order

117 papers	6,964 citations	53794 45 h-index	58581 82 g-index
117 all docs	117 docs citations	117 times ranked	3293 citing authors

#	Article	IF	Citations
1	How Proteins Trigger Excitation Energy Transfer in the FMO Complex of Green Sulfur Bacteria. Biophysical Journal, 2006, 91, 2778-2797.	0.5	592
2	Ultrafast excitation energy transfer dynamics in photosynthetic pigmentâ€“protein complexes. Physics Reports, 2001, 343, 137-254.	25.6	367
3	Intermolecular Coulomb Couplings from Ab Initio Electrostatic Potentials:â€‰ Application to Optical Transitions of Strongly Coupled Pigments in Photosynthetic Antennae and Reaction Centers. Journal of Physical Chemistry B, 2006, 110, 17268-17281.	2.6	348
4	On the relation of protein dynamics and exciton relaxation in pigmentâ€“protein complexes: An estimation of the spectral density and a theory for the calculation of optical spectra. Journal of Chemical Physics, 2002, 116, 9997-10019.	3.0	315
5	Photosystem II: The machinery of photosynthetic water splitting. Photosynthesis Research, 2008, 98, 53-80.	2.9	275
6	Quantum biology revisited. Science Advances, 2020, 6, eaaz4888.	10.3	266
7	Light Harvesting in Photosystem II Core Complexes Is Limited by the Transfer to the Trap:â€‰ Can the Core Complex Turn into a Photoprotective Mode?. Journal of the American Chemical Society, 2008, 130, 4431-4446.	13.7	197
8	Î±-Helices direct excitation energy flow in the Fennaâ€“Matthewsâ€“Olson protein. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 16862-16867.	7.1	183
9	The Eighth Bacteriochlorophyll Completes the Excitation Energy Funnel in the FMO Protein. Journal of Physical Chemistry Letters, 2011, 2, 93-98.	4.6	178
10	Theory of Optical Spectra of Photosystem II Reaction Centers: Location of the Triplet State and the Identity of the Primary Electron Donor. Biophysical Journal, 2005, 88, 986-998.	0.5	175
11	Calculation of pigment transition energies in the FMO protein. Photosynthesis Research, 2008, 95, 197-209.	2.9	170
12	Theory of excitation energy transfer: from structure to function. Photosynthesis Research, 2009, 102, 471-485.	2.9	158
13	Structure-Based Identification of Energy Sinks in Plant Light-Harvesting Complex II. Journal of Physical Chemistry B, 2010, 114, 13517-13535.	2.6	152
14	Understanding photosynthetic light-harvesting: a bottom up theoretical approach. Physical Chemistry Chemical Physics, 2013, 15, 3348-3371.	2.8	137
15	Spectroscopic Properties of Reaction Center Pigments in Photosystem II Core Complexes: Revision of the Multimer Model. Biophysical Journal, 2008, 95, 105-119.	0.5	133
16	Variable-Range Hopping Electron Transfer through Disordered Bridge States:Â Application to DNA. Journal of Physical Chemistry A, 2003, 107, 8404-8419.	2.5	132
17	Photosystem II Does Not Possess a Simple Excitation Energy Funnel: Time-Resolved Fluorescence Spectroscopy Meets Theory. Journal of the American Chemical Society, 2013, 135, 6903-6914.	13.7	107
18	Structure-Based Calculations of Optical Spectra of Photosystem I Suggest an Asymmetric Light-Harvesting Process. Journal of the American Chemical Society, 2010, 132, 3331-3343.	13.7	104

#	ARTICLE	IF	CITATIONS
19	Normal Mode Analysis of the Spectral Density of the Fennaâ€“Matthewsâ€“Olson Light-Harvesting Protein: How the Protein Dissipates the Excess Energy of Excitons. Journal of Physical Chemistry B, 2012, 116, 14565-14580.	2.6	102
20	Theory of Optical Spectra Involving Charge Transfer States: Dynamic Localization Predicts a Temperature Dependent Optical Band Shift. Physical Review Letters, 2004, 93, 188101.	7.8	99
21	Deciphering the Influence of Short-Range Electronic Couplings on Optical Properties of Molecular Dimers: Application to â€œSpecial Pairsâ€•in Photosynthesis. Journal of Physical Chemistry B, 2009, 113, 12603-12614.	2.6	93
22	Ultrafast Exciton Motion in Photosynthetic Antenna Systems:â€‰ The FMO-Complex. Journal of Physical Chemistry A, 1998, 102, 4381-4391.	2.5	91
23	Refinement of a Structural Model of a Pigmentâˆ'Protein Complex by Accurate Optical Line Shape Theory and Experiments. Journal of Physical Chemistry B, 2007, 111, 10487-10501.	2.6	88
24	Theory of exciton-vibrational dynamics in molecular dimers. Chemical Physics, 1996, 204, 99-114.	1.9	80
25	Crystal structure of cyanobacterial photosystem II at 3.0 Ã… resolution: A closer look at the antenna system and the small membrane-intrinsic subunits. Plant Physiology and Biochemistry, 2008, 46, 238-264.	5.8	80
26	Primary Photophysical Processes in Photosystem II: Bridging the Gap between Crystal Structure and Optical Spectra. ChemPhysChem, 2010, 11, 1141-1153.	2.1	76
27	Theory of excitonic couplings in dielectric media. Photosynthesis Research, 2012, 111, 47-52.	2.9	75
28	Challenges facing an understanding of the nature of low-energy excited states in photosynthesis. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1627-1640.	1.0	74
29	How the molecular structure determines the flow of excitation energy in plant light-harvesting complex II. Journal of Plant Physiology, 2011, 168, 1497-1509.	3.5	72
30	Simulations of Frequency-Domain Spectra: Structure-Function Relationships in Photosynthetic Pigment-Protein Complexes. Physical Review Letters, 2000, 84, 5228-5231.	7.8	64
31	Dissipative Exciton Motion in a Chlorophyll a/b Dimer of the Light Harvesting Complex of Photosystem II:â€‰ Simulation of Pumpâˆ'Probe Spectra. The Journal of Physical Chemistry, 1996, 100, 15654-15662.	2.9	61
32	Multiple Exciton Effects in Molecular Aggregates: Application to a Photosynthetic Antenna Complex. Physical Review Letters, 1997, 78, 3406-3409.	7.8	60
33	Photoionization of Xe inside<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>: Atom-fullerene hybridization, giant cross-section enhancement, and correlation confinement resonances. Physical Review A, 2010, 81, .	2.5	60
34	Photophysical Properties of PS-2 Reaction Centers and a Discrepancy in Exciton Relaxation Times. Journal of Physical Chemistry B, 2002, 106, 1809-1819.	2.6	56
35	Thermally Activated Superradiance and Intersystem Crossing in the Water-Soluble Chlorophyll Binding Protein. Journal of Physical Chemistry B, 2009, 113, 9948-9957.	2.6	56
36	Optical properties, excitation energy and primary charge transfer in photosystem II: Theory meets experiment. Journal of Photochemistry and Photobiology B: Biology, 2011, 104, 126-141.	3.8	56

#	Article	IF	Citations
37	Coupling to Charge Transfer States is the Key to Modulate the Optical Bands for Efficient Light Harvesting in Purple Bacteria. Journal of Physical Chemistry Letters, 2018, 9, 6892-6899.	4.6	55
38	Electrostatic Asymmetry in the Reaction Center of Photosystem II. Journal of Physical Chemistry Letters, 2017, 8, 850-858.	4.6	54
39	Theory of solvatochromic shifts in nonpolar solvents reveals a new spectroscopic rule. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13235-13240.	7.1	53
40	Towards an exact theory of linear absorbance and circular dichroism of pigment-protein complexes: Importance of non-secular contributions. Journal of Chemical Physics, 2015, 142, 034104.	3.0	52
41	The Primary Electron Donor of Photosystem II of the Cyanobacterium <i>Acaryochloris marina</i> Is a Chlorophyll <i>d</i> and the Water Oxidation Is Driven by a Chlorophyll <i>a</i>/Chlorophyll <i>d</i> Heterodimer. Journal of Physical Chemistry B, 2008, 112, 7351-7354.	2.6	50
42	Theory of Multiple Exciton Effects in the Photosynthetic Antenna Complex LHC-II. Journal of Physical Chemistry B, 1997, 101, 7232-7240.	2.6	48
43	Theory of excitation transfer in coupled nanostructures â€“ from quantum dots to light harvesting complexes. Physica Status Solidi (B): Basic Research, 2006, 243, 2302-2310.	1.5	48
44	Refined structure-based simulation of plant light-harvesting complex II: Linear optical spectra of trimers and aggregates. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, 1446-1460.	1.0	48
45	Pigmentâˆ’Pigment and Pigmentâˆ’Protein Interactions in Recombinant Water-Soluble Chlorophyll Proteins (WSCP) from Cauliflower. Journal of Physical Chemistry B, 2007, 111, 13325-13335.	2.6	47
46	Towards an ab initio description of the optical spectra of light-harvesting antennae: application to the CP29 complex of photosystem II. Physical Chemistry Chemical Physics, 2015, 17, 14405-14416.	2.8	47
47	Towards a structure-based exciton Hamiltonian for the CP29 antenna of photosystem II. Physical Chemistry Chemical Physics, 2014, 16, 11848-11863.	2.8	45
48	Site-directed Mutations at D1-Thr179 of Photosystem II in <i>Synechocystis</i> sp. PCC 6803 Modify the Spectroscopic Properties of the Accessory Chlorophyll in the D1-branch of the Reaction Center. Biochemistry, 2008, 47, 3143-3154.	2.5	44
49	Water soluble chlorophyll binding protein of higher plants: A most suitable model system for basic analyses of pigmentâ€“pigment and pigmentâ€“protein interactions in chlorophyll protein complexes. Journal of Plant Physiology, 2011, 168, 1462-1472.	3.5	44
50	Site-dependence of van der Waals interaction explains exciton spectra of double-walled tubular J-aggregates. Physical Chemistry Chemical Physics, 2015, 17, 6741-6747.	2.8	41
51	Structure-based modeling of energy transfer in photosynthesis. Photosynthesis Research, 2013, 116, 367-388.	2.9	40
52	Excited State Dynamics in Recombinant Water-Soluble Chlorophyll Proteins (WSCP) from Cauliflower Investigated by Transient Fluorescence Spectroscopy. Journal of Physical Chemistry B, 2008, 112, 13951-13961.	2.6	39
53	Structure-based simulation of linear optical spectra of the CP43 core antenna of photosystem II. Photosynthesis Research, 2012, 111, 87-101.	2.9	38
54	Circularly polarized luminescence spectroscopy reveals low-energy excited states and dynamic localization of vibronic transitions in CP43. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 115-128.	1.0	36

#	Article	IF	Citations
55	Theory of FRET â€œSpectroscopic Rulerâ€•for Short Distances: Application to Polyproline. Journal of Physical Chemistry B, 2018, 122, 54-67.	2.6	36
56	Long-Wavelength Limit of Photochemical Energy Conversion in Photosystem I. Journal of the American Chemical Society, 2014, 136, 3904-3918.	13.7	35
57	Structure Prediction of Self-Assembled Dye Aggregates from Cryogenic Transmission Electron Microscopy, Molecular Mechanics, and Theory of Optical Spectra. Journal of Physical Chemistry C, 2016, 120, 19416-19433.	3.1	35
58	Density Functional Studies of Iron-Porphyrin Cation with Small Ligands X (X: O, CO, NO,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 627 Td ((Physical Chemistry A, 2009, 113, 9202-9206.	2.5	34
59	Photoionization of hybrid states in endohedral fullerenes. Physical Review A, 2009, 79, .	2.5	30
60	The lowest-energy chlorophyll of photosystem II is adjacent to the peripheral antenna: Emitting states of CP47 assigned via circularly polarized luminescence. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1580-1593.	1.0	30
61	Ultrafast infrared observation of exciton equilibration from oriented single crystals of photosystem II. Nature Communications, 2016, 7, 13977.	12.8	26
62	Hole-Burning Spectroscopy on Excitonically Coupled Pigments in Proteins: Theory Meets Experiment. Journal of the American Chemical Society, 2016, 138, 2993-3001.	13.7	25
63	Lineshape theory of pigment-protein complexes: How the finite relaxation time of nuclei influences the exciton relaxation-induced lifetime broadening. Journal of Chemical Physics, 2016, 145, 034105.	3.0	24
64	A Bloch equation approach to intensity dependent optical spectra of light harvesting complex II. Photosynthesis Research, 2008, 95, 119-127.	2.9	23
65	Linear absorbance of the pheophorbide-a butanediamine dendrimer P4 in solution: Computational studies using a mixed quantum classical methodology. Journal of Chemical Physics, 2008, 128, 154905.	3.0	23
66	Excitonic effects in the lightâ€harvesting Chl a/bâ€“protein complex of higher plants. Physica Status Solidi (B): Basic Research, 1996, 194, 333-350.	1.5	22
67	The pheophorbide-a DAB dendrimer P4 in solution: MD-simulations based studies of exciton states. Chemical Physics Letters, 2007, 444, 118-124.	2.6	22
68	Calculating Optical Absorption Spectra of Thin Polycrystalline Organic Films: Structural Disorder and Site-Dependent van der Waals Interaction. Journal of Physical Chemistry C, 2015, 119, 5747-5751.	3.1	22
69	Origin of non-conservative circular dichroism of the CP29 antenna complex of photosystem II. Physical Chemistry Chemical Physics, 2017, 19, 7524-7536.	2.8	22
70	Interhelical interactions within the STIM1 CC1 domain modulate CRAC channel activation. Nature Chemical Biology, 2021, 17, 196-204.	8.0	22
71	Site-directed mutations at D1-His198 and D1-Thr179 of photosystem II in <i>Synechocystis</i> sp. PCC 6803: deciphering the spectral properties of the PSII reaction centre. Philosophical Transactions of the Royal Society B: Biological Sciences, 2008, 363, 1197-1202.	4.0	21
72	Mixed Quantumâ€Classical Description of Excitation Energy Transfer in Supramolecular Complexes: Screening of the Excitonic Coupling. ChemPhysChem, 2014, 15, 478-485.	2.1	21

#	Article	IF	Citations
73	The quest for energy traps in the CP43 antenna of photosystem II. Journal of Photochemistry and Photobiology B: Biology, 2015, 152, 286-300.	3.8	21
74	Influence of Higher Excited Singlet States on Ultrafast Exciton Motion in Pigmentâ€Protein Complexes. Photochemistry and Photobiology, 1997, 66, 618-627.	2.5	20
75	Revealing the Functional States in the Active Site of BLUF Photoreceptors from Electrochromic Shift Calculations. Journal of Physical Chemistry B, 2014, 118, 11109-11119.	2.6	20
76	Theory of Anisotropic Circular Dichroism of Excitonically Coupled Systems: Application to the Baseplate of Green Sulfur Bacteria. Journal of Physical Chemistry B, 2018, 122, 2747-2756.	2.6	20
77	Towards a quantitative description of excitonic couplings in photosynthetic pigmentâ€“protein complexes: quantum chemistry driven multiscale approaches. Physical Chemistry Chemical Physics, 2022, 24, 5014-5038.	2.8	20
78	Nonperturbative theory for the optical response to strong light of the light harvesting complex II of plants: Saturation of the fluorescence quantum yield. Journal of Chemical Physics, 2007, 127, 075105.	3.0	19
79	Anisotropic Circular Dichroism of Light-Harvesting Complex II in Oriented Lipid Bilayers: Theory Meets Experiment. Journal of Physical Chemistry B, 2019, 123, 1090-1098.	2.6	18
80	Static Disorder in Excitation Energies of the Fennaâ€“Matthewsâ€“Olson Protein: Structure-Based Theory Meets Experiment. Journal of Physical Chemistry Letters, 2020, 11, 10306-10314.	4.6	16
81	Structure-Based Theory of Fluctuation-Induced Energy Transfer in a Molecular Dyad. Journal of Physical Chemistry Letters, 2018, 9, 5940-5947.	4.6	15
82	Semiclassical Modified Redfield and Generalized FÃ¶rster Theories of Exciton Relaxation/Transfer in Light-Harvesting Complexes: The Quest for the Principle of Detailed Balance. Journal of Physical Chemistry B, 2021, 125, 6406-6416.	2.6	14
83	Exact simulation of pigment-protein complexes unveils vibronic renormalization of electronic parameters in ultrafast spectroscopy. Nature Communications, 2022, 13, .	12.8	14
84	Red/Green Color Tuning of Visual Rhodopsins: Electrostatic Theory Provides a Quantitative Explanation. Journal of Physical Chemistry B, 2018, 122, 4828-4837.	2.6	13
85	Theory of linear absorption spectra of biological and non-biological chromophore complexes. Chemical Physics, 2002, 275, 333-354.	1.9	12
86	Defects in the STIM1 SOARÎ±2 domain affect multiple steps in the CRAC channel activation cascade. Cellular and Molecular Life Sciences, 2021, 78, 6645-6667.	5.4	12
87	Normal mode analysis of spectral density of FMO trimers: Intra- and intermonomer energy transfer. Journal of Chemical Physics, 2020, 153, 215103.	3.0	11
88	Theory of Excitation Energy Transfer and Optical Spectra of Photosynthetic Systems. Advances in Photosynthesis and Respiration, 2008, , 421-443.	1.0	10
89	Anharmonic Oscillator Approach to the Excitonâ€Exciton Annihilation Dynamics in Molecular Aggregates. Journal of the Chinese Chemical Society, 2000, 47, 807-819.	1.4	9
90	Variation of Exciton-Vibrational Coupling in Photosystem II Core Complexes from <i>Thermosynechococcus elongatus</i> As Revealed by Single-Molecule Spectroscopy. Journal of Physical Chemistry B, 2015, 119, 4203-4210.	2.6	9

#	Article	IF	Citations
91	Modeling of Optical Spectra and Light Harvesting in Photosystem I. , 2006, , 595-610.		8
92	Line Narrowing of Excited-State Transitions in Nonlinear Polarization Spectroscopy: Application to Water-Soluble Chlorophyll-Binding Protein. Physical Review Letters, 2012, 108, 178104.	7.8	7
93	Chapter 2. Absorption of Light, Excitation Energy Transfer and Electron Transfer Reactions. Comprehensive Series in Photochemical and Photobiological Sciences, 2007, , 39-97.	0.3	6
94	Structure-Based Calculation of Pigmentâ€“Protein and Excitonic Pigmentâ€“Pigment Coupling in Photosynthetic Light-Harvesting Complexes. , 2014, , 3-44.		6
95	Theory of sub-picosecond exciton motion in photosynthetic antenna systems. Applied Physics B: Lasers and Optics, 2000, 71, 451-456.	2.2	4
96	Qualitative change of character of dispersive interaction with intermolecular distance. Journal of Chemical Physics, 2013, 139, 044103.	3.0	4
97	Comparative theoretical studies on exciton dynamics in biological and artificial chromophore complexes. Journal of Luminescence, 2000, 87-89, 803-805.	3.1	3
98	A New Spectroscopic Tool for Analyzing Excitonic Structure and Dynamics in Pigment-Protein Complexes. Biophysical Journal, 2008, 95, 495-496.	0.5	3
99	Reply to â€œComment on â€˜Calculating Optical Absorption Spectra of Thin Polycrystalline Organic Films: Structural Disorder and Site-Dependent van der Waals Interactionâ€™â€. Journal of Physical Chemistry C, 2015, 119, 18818-18820.	3.1	3
100	Wavelength-Dependent Excitonâ€“Vibrational Coupling in the Water-Soluble Chlorophyll Binding Protein Revealed by Multilevel Theory of Difference Fluorescence Line-Narrowing. Journal of Physical Chemistry B, 2018, 122, 8891-8899.	2.6	3
101	Non-conservative circular dichroism of photosystem II reaction centers: Is there an enhancement by a coupling with charge transfer states?. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 404, 112883.	3.9	3
102	Modeling of photosynthetic light-harvesting: From structure to function. Procedia Chemistry, 2011, 3, 236-247.	0.7	2
103	ARGOS: An adaptive refinement goalâ€oriented solver for the linearized Poissonâ€“Boltzmann equation. Journal of Computational Chemistry, 2021, 42, 1832-1860.	3.3	2
104	Low Quantum Yield Electron Transfer Pathways in PSII. , 2008, , 191-195.		1
105	Femtosecond Infrared Crystallography of Photosystem II Core Complexes: Watching Exciton Dynamics and Charge Separation in Real Space and Time. , 2017, , 81-116.		1
106	Structural determinants of a permeation barrier of the SecYEG translocon in the active state. Physical Chemistry Chemical Physics, 2021, 23, 25830-25840.	2.8	1
107	Photo-induced ultrafast transfer phenomena in molecular complexes. Journal of Luminescence, 1998, 76-77, 365-367.	3.1	0
108	Theory of Ultrafast Exciton Motion in Photosynthetic Antenna Systems. Molecular Crystals and Liquid Crystals, 1998, 324, 31-36.	0.3	0

#	Article	IF	Citations
109	Linear and nonlinear optics of light harvesting complexes: TCL- and Bloch Equations for linear spectra and saturation dynamics. , 2007, , .		0
110	Optical Bloch equations for light harvesting complexes: pump probe spectra and saturation dynamics at high light intensity excitation. , 2009, , .		0
111	Discussions on Session 2B:Quantum effects in chemistry. Procedia Chemistry, 2011, 3, 118-121.	0.7	0
112	Discussions on Session 3A:Quantum dynamic theory. Procedia Chemistry, 2011, 3, 165-171.	0.7	0
113	Discussions on Session 3B:Quantum dynamic theory. Procedia Chemistry, 2011, 3, 185-187.	0.7	0
114	Discussions on Session 4A:Quantum effects in biology: photosynthesis. Procedia Chemistry, 2011, 3, 232-235.	0.7	0
115	Photophysics of Photosynthetic Reaction Centres. RSC Energy and Environment Series, 2011, , 143-162.	0.5	0
116	Theory of Line Narrowing in Nonlinear Polarization Spectroscopy. , 2012, , .		0
117	Equilibration of Excitons and Double Excited Light Harvesting Complex of Photosystem II. , 1995, , 243-246.		0