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	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
2	Exact simulation of pigment-protein complexes unveils vibronic renormalization of electronic parameters in ultrafast spectroscopy. Nature Communications, 2022, 13, .	12.8	14
3	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
4	Interhelical interactions within the STIM1 CC1 domain modulate CRAC channel activation. Nature Chemical Biology, 2021, 17, 196-204.	8.0	22
5	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
6	ARGOS: An adaptive refinement goalâ€oriented solver for the linearized Poissonâ€“Boltzmann equation. Journal of Computational Chemistry, 2021, 42, 1832-1860.	3.3	2
7	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
8	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
9	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
10	Quantum biology revisited. Science Advances, 2020, 6, eaaz4888.	10.3	266
11	Normal mode analysis of spectral density of FMO trimers: Intra- and intermonomer energy transfer. Journal of Chemical Physics, 2020, 153, 215103.	3.0	11
12	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
13	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
14	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
15	Theory of FRET â€œSpectroscopic Rulerâ€•for Short Distances: Application to Polyproline. Journal of Physical Chemistry B, 2018, 122, 54-67.	2.6	36
16	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
17	Structure-Based Theory of Fluctuation-Induced Energy Transfer in a Molecular Dyad. Journal of Physical Chemistry Letters, 2018, 9, 5940-5947.	4.6	15
18	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

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19	Electrostatic Asymmetry in the Reaction Center of Photosystem II. Journal of Physical Chemistry Letters, 2017, 8, 850-858.	4.6	54
20	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
21	Femtosecond Infrared Crystallography of Photosystem II Core Complexes: Watching Exciton Dynamics and Charge Separation in Real Space and Time. , 2017, , 81-116.		1
22	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
23	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
24	Ultrafast infrared observation of exciton equilibration from oriented single crystals of photosystem II. Nature Communications, 2016, 7, 13977.	12.8	26
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	Structure-Based Calculation of Pigmentâ€“Protein and Excitonic Pigmentâ€“Pigment Coupling in Photosynthetic Light-Harvesting Complexes. , 2014, , 3-44.		6

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37	Long-Wavelength Limit of Photochemical Energy Conversion in Photosystem I. Journal of the American Chemical Society, 2014, 136, 3904-3918.	13.7	35
38	Towards a structure-based exciton Hamiltonian for the CP29 antenna of photosystem II. Physical Chemistry Chemical Physics, 2014, 16, 11848-11863.	2.8	45
39	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
40	Mixed Quantumâ€Classical Description of Excitation Energy Transfer in Supramolecular Complexes: Screening of the Excitonic Coupling. ChemPhysChem, 2014, 15, 478-485.	2.1	21
41	Qualitative change of character of dispersive interaction with intermolecular distance. Journal of Chemical Physics, 2013, 139, 044103.	3.0	4
42	Structure-based modeling of energy transfer in photosynthesis. Photosynthesis Research, 2013, 116, 367-388.	2.9	40
43	Understanding photosynthetic light-harvesting: a bottom up theoretical approach. Physical Chemistry Chemical Physics, 2013, 15, 3348-3371.	2.8	137
44	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
45	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
46	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
47	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
48	Structure-based simulation of linear optical spectra of the CP43 core antenna of photosystem II. Photosynthesis Research, 2012, 111, 87-101.	2.9	38
49	Theory of excitonic couplings in dielectric media. Photosynthesis Research, 2012, 111, 47-52.	2.9	75
50	Theory of Line Narrowing in Nonlinear Polarization Spectroscopy. , 2012, , .		0
51	The Eighth Bacteriochlorophyll Completes the Excitation Energy Funnel in the FMO Protein. Journal of Physical Chemistry Letters, 2011, 2, 93-98.	4.6	178
52	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
53	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
54	Discussions on Session 2B:Quantum effects in chemistry. Procedia Chemistry, 2011, 3, 118-121.	0.7	0

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55	Discussions on Session 3A:Quantum dynamic theory. Procedia Chemistry, 2011, 3, 165-171.	0.7	0
56	Discussions on Session 3B:Quantum dynamic theory. Procedia Chemistry, 2011, 3, 185-187.	0.7	0
57	Discussions on Session 4A:Quantum effects in biology: photosynthesis. Procedia Chemistry, 2011, 3, 232-235.	0.7	0
58	Modeling of photosynthetic light-harvesting: From structure to function. Procedia Chemistry, 2011, 3, 236-247.	0.7	2
59	Photophysics of Photosynthetic Reaction Centres. RSC Energy and Environment Series, 2011, , 143-162.	0.5	0
60	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
61	Primary Photophysical Processes in Photosystem II: Bridging the Gap between Crystal Structure and Optical Spectra. ChemPhysChem, 2010, 11, 1141-1153.	2.1	76
62	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
63	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
64	Structure-Based Identification of Energy Sinks in Plant Light-Harvesting Complex II. Journal of Physical Chemistry B, 2010, 114, 13517-13535.	2.6	152
65	Photoionization of hybrid states in endohedral fullerenes. Physical Review A, 2009, 79, .	2.5	30
66	Theory of excitation energy transfer: from structure to function. Photosynthesis Research, 2009, 102, 471-485.	2.9	158
67	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
68	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
69	Density Functional Studies of Iron-Porphyrin Cation with Small Ligands X (X: O, CO, NO,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Physical Chemistry A, 2009, 113, 9202-9206.	2.5	34
70	Optical Bloch equations for light harvesting complexes: pump probe spectra and saturation dynamics at high light intensity excitation. , 2009, , .		0
71	Calculation of pigment transition energies in the FMO protein. Photosynthesis Research, 2008, 95, 197-209.	2.9	170
72	A Bloch equation approach to intensity dependent optical spectra of light harvesting complex II. Photosynthesis Research, 2008, 95, 119-127.	2.9	23

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73	Photosystem II: The machinery of photosynthetic water splitting. Photosynthesis Research, 2008, 98, 53-80.	2.9	275
74	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
75	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
76	A New Spectroscopic Tool for Analyzing Excitonic Structure and Dynamics in Pigment-Protein Complexes. Biophysical Journal, 2008, 95, 495-496.	0.5	3
77	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
78	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
79	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
80	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
81	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
82	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
83	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
84	Low Quantum Yield Electron Transfer Pathways in PSII. , 2008, , 191-195.		1
85	Theory of Excitation Energy Transfer and Optical Spectra of Photosynthetic Systems. Advances in Photosynthesis and Respiration, 2008, , 421-443.	1.0	10
86	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
87	Linear and nonlinear optics of light harvesting complexes: TCL- and Bloch Equations for linear spectra and saturation dynamics. , 2007, , .		0
88	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
89	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
90	Pigmentâ^'Pigment and Pigmentâ^'Protein Interactions in Recombinant Water-Soluble Chlorophyll Proteins (WSCP) from Cauliflower. Journal of Physical Chemistry B, 2007, 111, 13325-13335.	2.6	47

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91	Refinement of a Structural Model of a Pigmentâ˘Protein Complex by Accurate Optical Line Shape Theory and Experiments. Journal of Physical Chemistry B, 2007, 111, 10487-10501.	2.6	88
92	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
93	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
94	How Proteins Trigger Excitation Energy Transfer in the FMO Complex of Green Sulfur Bacteria. Biophysical Journal, 2006, 91, 2778-2797.	0.5	592
95	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
96	Modeling of Optical Spectra and Light Harvesting in Photosystem I. , 2006, , 595-610.		8
97	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
98	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
99	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
100	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
101	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
102	Theory of linear absorption spectra of biological and non-biological chromophore complexes. Chemical Physics, 2002, 275, 333-354.	1.9	12
103	Ultrafast excitation energy transfer dynamics in photosynthetic pigmentâ€“protein complexes. Physics Reports, 2001, 343, 137-254.	25.6	367
104	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
105	Comparative theoretical studies on exciton dynamics in biological and artificial chromophore complexes. Journal of Luminescence, 2000, 87-89, 803-805.	3.1	3
106	Theory of sub-picosecond exciton motion in photosynthetic antenna systems. Applied Physics B: Lasers and Optics, 2000, 71, 451-456.	2.2	4
107	Simulations of Frequency-Domain Spectra: Structure-Function Relationships in Photosynthetic Pigment-Protein Complexes. Physical Review Letters, 2000, 84, 5228-5231.	7.8	64
108	Photo-induced ultrafast transfer phenomena in molecular complexes. Journal of Luminescence, 1998, 76-77, 365-367.	3.1	0

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109	Ultrafast Exciton Motion in Photosynthetic Antenna Systems:â€‰ The FMO-Complex. Journal of Physical Chemistry A, 1998, 102, 4381-4391.	2.5	91
110	Theory of Ultrafast Exciton Motion in Photosynthetic Antenna Systems. Molecular Crystals and Liquid Crystals, 1998, 324, 31-36.	0.3	0
111	Multiple Exciton Effects in Molecular Aggregates: Application to a Photosynthetic Antenna Complex. Physical Review Letters, 1997, 78, 3406-3409.	7.8	60
112	Theory of Multiple Exciton Effects in the Photosynthetic Antenna Complex LHC-II. Journal of Physical Chemistry B, 1997, 101, 7232-7240.	2.6	48
113	Influence of Higher Excited Singlet States on Ultrafast Exciton Motion in Pigmentâ€Protein Complexes. Photochemistry and Photobiology, 1997, 66, 618-627.	2.5	20
114	Theory of exciton-vibrational dynamics in molecular dimers. Chemical Physics, 1996, 204, 99-114.	1.9	80
115	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
116	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
117	Equilibration of Excitons and Double Excited Light Harvesting Complex of Photosystem II. , 1995, , 243-246.		0