David R Klug

List of Publications by Year
in descending order

103 papers	9,305 citations	57758 44 h-index	45317 90 g-index
107 all docs	107 docs citations	107 times ranked	8525 citing authors

#	Article	IF	Citations
1	Mechanism of Photocatalytic Water Splitting in TiO₂. Reaction of Water with Photoholes, Importance of Charge Carrier Dynamics, and Evidence for Four-Hole Chemistry. Journal of the American Chemical Society, 2008, 130, 13885-13891.	13.7	850
2	Subpicosecond Interfacial Charge Separation in Dye-Sensitized Nanocrystalline Titanium Dioxide Films. The Journal of Physical Chemistry, 1996, 100, 20056-20062.	2.9	815
3	Parameters Influencing Charge Recombination Kinetics in Dye-Sensitized Nanocrystalline Titanium Dioxide Films. Journal of Physical Chemistry B, 2000, 104, 538-547.	2.6	613
4	The Role of Cobalt Phosphate in Enhancing the Photocatalytic Activity of Î±-Fe₂O₃ toward Water Oxidation. Journal of the American Chemical Society, 2011, 133, 14868-14871.	13.7	533
5	Charge Separation versus Recombination in Dye-Sensitized Nanocrystalline Solar Cells:Â the Minimization of Kinetic Redundancy. Journal of the American Chemical Society, 2005, 127, 3456-3462.	13.7	477
6	Electron Injection and Recombination in Dye Sensitized Nanocrystalline Titanium Dioxide Films:â€‰ A Comparison of Ruthenium Bipyridyl and Porphyrin Sensitizer Dyes. Journal of Physical Chemistry B, 2000, 104, 1198-1205.	2.6	433
7	Dynamics of photogenerated holes in surface modified Î±-Fe ₂ O ₃ photoanodes for solar water splitting. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15640-15645.	7.1	413
8	Trap-limited recombination in dye-sensitized nanocrystalline metal oxide electrodes. Physical Review B, 2001, 63, .	3.2	378
9	Charge Recombination Kinetics in Dye-Sensitized Nanocrystalline Titanium Dioxide Films under Externally Applied Bias. Journal of Physical Chemistry B, 1998, 102, 1745-1749.	2.6	334
10	Dynamics of photogenerated holes in nanocrystalline Î±-Fe₂O₃electrodes for water oxidation probed by transient absorption spectroscopy. Chemical Communications, 2011, 47, 716-718.	4.1	261
11	Activation Energies for the Rate-Limiting Step in Water Photooxidation by Nanostructured Î±-Fe₂O₃ and TiO₂. Journal of the American Chemical Society, 2011, 133, 10134-10140.	13.7	247
12	Water Splitting by Nanocrystalline TiO₂ in a Complete Photoelectrochemical Cell Exhibits Efficiencies Limited by Charge Recombination. Journal of Physical Chemistry C, 2010, 114, 4208-4214.	3.1	228
13	Efficient Suppression of Electronâ€“Hole Recombination in Oxygen-Deficient Hydrogen-Treated TiO₂ Nanowires for Photoelectrochemical Water Splitting. Journal of Physical Chemistry C, 2013, 117, 25837-25844.	3.1	222
14	Correlating long-lived photogenerated hole populations with photocurrent densities in hematite water oxidation photoanodes. Energy and Environmental Science, 2012, 5, 6304-6312.	30.8	196
15	Charge Separation in Solid-State Dye-Sensitized Heterojunction Solar Cells. Journal of the American Chemical Society, 1999, 121, 7445-7446.	13.7	195
16	Modulation of the Rate of Electron Injection in Dye-Sensitized Nanocrystalline TiO2Films by Externally Applied Bias. Journal of Physical Chemistry B, 2001, 105, 7424-7431.	2.6	171
17	Charge Carrier Dynamics on Mesoporous WO₃ during Water Splitting. Journal of Physical Chemistry Letters, 2011, 2, 1900-1903.	4.6	142
18	Mechanism of O₂ Production from Water Splitting: Nature of Charge Carriers in Nitrogen Doped Nanocrystalline TiO₂ Films and Factors Limiting O₂ Production. Journal of Physical Chemistry C, 2011, 115, 3143-3150.	3.1	123

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19	Comment on â€œMeasurement of Ultrafast Photoinduced Electron Transfer from Chemically Anchored Ruâ”Dye Molecules into Empty Electronic States in a Colloidal Anatase TiO2Filmâ€• Journal of Physical Chemistry B, 1998, 102, 3649-3650.	2.6	114
20	Proton/Hydrogen Transfer Affects the S-State-Dependent Microsecond Phases of P680+ Reduction during Water Splitting. Biochemistry, 1998, 37, 3974-3981.	2.5	114
21	The state of detergent solubilised light-harvesting chlorophyll-a/b protein complex as monitored by picosecond time-resolved fluorescence and circular dichroism. Biochimica Et Biophysica Acta - Bioenergetics, 1987, 893, 349-364.	1.0	110
22	A first step towards practical single cell proteomics: a microfluidic antibody capture chip with TIRF detection. Lab on A Chip, 2011, 11, 1256.	6.0	105
23	Exciton Equilibration Induced by Phonons:â€‰ Theory and Application to PS II Reaction Centers. Journal of Physical Chemistry B, 1997, 101, 7205-7210.	2.6	101
24	Observation of pheophytin reduction in photosystem two reaction centers using femtosecond transient absorption spectroscopy. Biochemistry, 1992, 31, 7638-7647.	2.5	100
25	Sensing isothermal changes in the lateral pressure in model membranes using di-pyrenyl phosphatidylcholine. Faraday Discussions, 1999, 111, 41-53.	3.2	96
26	Electron injection kinetics for the nanocrystalline TiO2 films sensitised with the dye (Bu4N)2Ru(dcbpyH)2(NCS)2. Chemical Physics, 2002, 285, 127-132.	1.9	95
27	Oxygen deficient Î±-Fe₂O₃ photoelectrodes: a balance between enhanced electrical properties and trap-mediated losses. Chemical Science, 2015, 6, 4009-4016.	7.4	92
28	Observation of multiple radical pair states in photosystem 2 reaction centers. Biochemistry, 1991, 30, 7573-7586.	2.5	87
29	Modulation of Quantum Yield of Primary Radical Pair Formation in Photosystem II by Site-Directed Mutagenesis Affecting Radical Cations and Anions. Biochemistry, 1998, 37, 17439-17447.	2.5	87
30	Large and Fast Relaxations inside a Protein:Â Calculation and Measurement of Reorganization Energies in Alcohol Dehydrogenase. Journal of Physical Chemistry B, 2002, 106, 11658-11665.	2.6	86
31	Transient luminescence studies of electron injection in dye sensitised nanocrystalline TiO2 films. Journal of Photochemistry and Photobiology A: Chemistry, 2001, 142, 215-220.	3.9	82
32	Acoustic suppression of the coffee-ring effect. Soft Matter, 2015, 11, 7207-7213.	2.7	79
33	A quantitative structure-function relationship for the Photosystem II reaction center: Supermolecular behavior in natural photosynthesis. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 946-951.	7.1	75
34	Comparison of Primary Charge Separation in the Photosystem II Reaction Center Complex Isolated from Wild-type and D1-130 Mutants of the Cyanobacterium Synechocystis PCC 6803. Journal of Biological Chemistry, 1996, 271, 2093-2101.	3.4	74
35	Primary processes in isolated Photosystem II reaction centres probed by magic angle transient absorption spectroscopy. Chemical Physics, 1995, 194, 433-442.	1.9	60
36	Charge carrier separation in nanostructured TiO2 photoelectrodes for water splitting. Physical Chemistry Chemical Physics, 2013, 15, 8772.	2.8	58

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37	A Quantum Mechanical/Molecular Mechanical Approach to Relaxation Dynamics:â€‰ Calculation of the Optical Properties of Solvated Bacteriochlorophyll-a. Journal of Physical Chemistry B, 1999, 103, 7720-7727.	2.6	56
38	Interfacial charge separation in Cu₂O/RuO_x as a visible light driven CO₂ reduction catalyst. Physical Chemistry Chemical Physics, 2014, 16, 5922-5926.	2.8	55
39	Biological and Biomedical Applications of Two-Dimensional Vibrational Spectroscopy: Proteomics, Imaging, and Structural Analysis. Accounts of Chemical Research, 2009, 42, 1322-1331.	15.6	53
40	Rate of oxidation of P680 in isolated photosystem 2 reaction centers monitored by loss of chlorophyll stimulated emission. Biochemistry, 1993, 32, 8259-8267.	2.5	50
41	Protein identification and quantification by two-dimensional infrared spectroscopy: Implications for an all-optical proteomic platform. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 15352-15357.	7.1	50
42	Does Slow Energy Transfer Limit the Observed Time Constant for Radical Pair Formation in Photosystem II Reaction Centers?. Biochemistry, 1994, 33, 14768-14774.	2.5	48
43	Determination of P680 singlet state lifetimes in photosystem two reaction centres. Chemical Physics Letters, 1992, 188, 54-60.	2.6	45
44	Sub-picosecond Equilibration of Excitation Energy in Isolated Photosystem II Reaction Centers Revisited:â€‰ Time-Dependent Anisotropy. The Journal of Physical Chemistry, 1996, 100, 10469-10478.	2.9	45
45	Relationship between Excitation Energy Transfer, Trapping, and Antenna Size in Photosystem II. Biochemistry, 2001, 40, 4026-4034.	2.5	39
46	The Temperature Dependence of P680+ Reduction in Oxygen-Evolving Photosystem II. Biochemistry, 2002, 41, 5015-5023.	2.5	35
47	Chemical-Free Lysis and Fractionation of Cells by Use of Surface Acoustic Waves for Sensitive Protein Assays. Analytical Chemistry, 2015, 87, 2161-2169.	6.5	34
48	Direct identification and decongestion of Fermi resonances by control of pulse time ordering in two-dimensional IR spectroscopy. Journal of Chemical Physics, 2007, 127, 114513.	3.0	33
49	Quantitative single cell and single molecule proteomics for clinical studies. Current Opinion in Biotechnology, 2013, 24, 745-751.	6.6	33
50	Optical fingerprinting of peptides using two-dimensional infrared spectroscopy: Proof of principle. Analytical Biochemistry, 2008, 374, 358-365.	2.4	31
51	A microfluidic platform for probing single cell plasma membranes using optically trapped Smart Droplet Microtools (SDMs). Lab on A Chip, 2009, 9, 1096.	6.0	27
52	Detection of complex formation and determination of intermolecular geometry through electrical anharmonic coupling of molecular vibrations using electron-vibrationâ€“vibration two-dimensional infrared spectroscopy. Physical Chemistry Chemical Physics, 2009, 11, 8417.	2.8	27
53	Scaling advantages and constraints in miniaturized capture assays for single cell protein analysis. Lab on A Chip, 2013, 13, 2066.	6.0	25
54	The entanglement of excitation energy transfer and electron transfer in the reaction centre of photosystem II. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 1998, 356, 449-464.	3.4	24

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55	Decongestion of methylene spectra in biological and non-biological systems using picosecond 2DIR spectroscopy measuring electron-vibrationâ€“vibration coupling. Chemical Physics, 2008, 350, 201-211.	1.9	23
56	Optical properties of solvated molecules calculated by a QMMM method Chlorophyll a and bacteriochlorophyll a. Faraday Discussions, 1997, 108, 51-62.	3.2	20
57	Unfolding Energetics of G-Î±-Actin: A Discrete Intermediate can be Re-folded to the Native State by CCT. Journal of Molecular Biology, 2005, 353, 385-396.	4.2	19
58	Comparison of basis set effects and the performance ofab initio and DFT methods for probing equilibrium fluctuations. Journal of Computational Chemistry, 2007, 28, 478-490.	3.3	19
59	Absolute quantification of protein copy number using a single-molecule-sensitive microarray. Analyst, The, 2014, 139, 3235.	3.5	19
60	Repurposed floxacins targeting RSK4 prevent chemoresistance and metastasis in lung and bladder cancer. Science Translational Medicine, 2021, 13, .	12.4	19
61	Identification and Relative Quantification of Tyrosine Nitration in a Model Peptide Using Two-Dimensional Infrared Spectroscopy. Journal of Physical Chemistry B, 2014, 118, 12855-12864.	2.6	16
62	Geometry determination of complexes in a molecular liquid mixture using electronâ€“vibrationâ€“vibration two-dimensional infrared spectroscopy with a vibrational transition density cube method. Physical Chemistry Chemical Physics, 2012, 14, 14023.	2.8	13
63	Addressable droplet microarrays for single cell protein analysis. Analyst, The, 2014, 139, 5367-5374.	3.5	13
64	Multiplexed single cell protein expression analysis in solid tumours using a miniaturised microfluidic assay. Convergent Science Physical Oncology, 2017, 3, 024003.	2.6	13
65	Redox potentials of cytochrome b-559 in the D1/D2/cytochrome b-559 reaction centre of Photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 1993, 1143, 239-242.	1.0	12
66	Comparison of primary electron transfer in Photosystem II reaction centres isolated from the higher plant Pisum sativum and the green alga Chlamydomonas reinhardtii. Biochimica Et Biophysica Acta - Bioenergetics, 1994, 1186, 247-251.	1.0	12
67	Picosecond time-resolved absorption and emission studies of pyrazolotriazole azomethine dyes. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 3479.	1.7	10
68	Dephasing of excited-state wave packets in an oxazine dye. The Journal of Physical Chemistry, 1993, 97, 12561-12565.	2.9	10
69	The grab-and-drop protocol: a novel strategy for membrane protein isolation and reconstitution from single cells. Analyst, The, 2014, 139, 3296-3304.	3.5	10
70	Absolute Measurement of Phosphorylation Levels in a Biological Membrane Using Atomic Force Microscopy:â€‰ The Creation of Phosphorylation Maps. Biochemistry, 2002, 41, 8535-8539.	2.5	9
71	Detection of Drug Binding to a Target Protein Using EVV 2DIR Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 3598-3606.	2.6	9
72	Two-Dimensional Partial-Covariance Mass Spectrometry of Large Molecules Based on Fragment Correlations. Physical Review X, 2020, 10, .	8.9	9

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73	The design of a picosecond flash spectroscope and its application to photosynthesis. Journal of the Chemical Society, Faraday Transactions 2, 1986, 82, 2111.	1.1	7
74	Picosecond absorption spectroscopy of Photosystem I reaction centres from higher plants. Biochemical Society Transactions, 1986, 14, 47-48.	3.4	7
75	Title is missing!. Photosynthesis Research, 1999, 60, 191-198.	2.9	7
76	Potential for the detection of molecular complexes and determination of interaction geometry by 2DIR: Application to protein sciences. Faraday Discussions, 2011, 150, 161.	3.2	7
77	Energy Trapping and Equilibration: A Balance of Regulation and Efficiency. Advances in Photosynthesis and Respiration, 2005, , 491-514.	1.0	7
78	Effect of Adiabaticity on Electron Dynamics in Zinc Myoglobin. Journal of Physical Chemistry B, 2005, 109, 5954-5961.	2.6	6
79	A Novel Aî²40 Assembly at Physiological Concentration. Scientific Reports, 2020, 10, 9477.	3.3	6
80	Generation of Simplified Protein Raman Spectra Using Three-Color Picosecond Coherent Anti-Stokes Raman Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 12175-12181.	2.6	5
81	Protein degradation rate is the dominant mechanism accounting for the differences in protein abundance of basal p53 in a human breast and colorectal cancer cell line. PLoS ONE, 2017, 12, e0177336.	2.5	5
82	Evaluation of FOXO1 Target Engagement Using a Single-Cell Microfluidic Platform. Analytical Chemistry, 2021, 93, 14659-14666.	6.5	5
83	Title is missing!. Photosynthesis Research, 1999, 62, 205-217.	2.9	4
84	Picosecond fluorescence and absorption spectroscopy of light-harvesting chlorophyll-protein complex from pea chloroplasts. Biochemical Society Transactions, 1986, 14, 34-34.	3.4	3
85	A unified picture of energy and electron transfer in primary photosynthesis. Chemical Physics, 2005, 319, 308-315.	1.9	3
86	Small-molecule optical probes for cell imaging of protein sulfenylation and their application to monitor cisplatin induced protein oxidation. Sensors and Actuators B: Chemical, 2017, 248, 437-446.	7.8	3
87	Affinity chromatography and capillary electrophoresis for analysis of the yeast ribosomal proteins. BMB Reports, 2012, 45, 233-238.	2.4	3
88	Trapping of excitation energy by photosystem two reaction centres: Is P680 a multimer?. Solar Energy Materials and Solar Cells, 1995, 38, 135-138.	6.2	2
89	A Quantum Mechanical/Molecular Mechanical Approach to Solvation Dynamics Tested by Three Pulse Photon Echo Measurements. Springer Series in Chemical Physics, 1998, , 532-534.	0.2	2
90	The Influence of Energy Level Disorder on the Charge Separation / Trapping Kinetics in Photosystem Two. , 1995, , 611-614.		2

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91	Identification of Chlorophyll Anion States During Charge Separation in Mutant Photosystem II Reaction Centres. , 1998, , 1041-1044.		2
92	Abstract 1775: Targeting RSK4 prevents both chemoresistance and metastasis in lung cancer. , 2019, , .		2
93	A comparison of the photochemical activity of two forms of Photosystem II reaction centre isolated from sugar beet. Biochimica Et Biophysica Acta - Bioenergetics, 1994, 1185, 85-91.	1.0	1
94	Detergent effects upon the picosecond dynamics of higher-plant light-harvesting chlorophyll complex (LHC2). Journal of the Chemical Society, Faraday Transactions 2, 1986, 82, 2263.	1.1	0
95	EUV light source and laser considerations for scalability and high-energy conversion efficiency. , 2002, , .		0
96	Does History Repeat Itself? The Emergence of a New Discipline. ACS Chemical Biology, 2006, 1, 737-740.	3.4	0
97	Detection of Molecular Complex Formation and Direct Determination of Intermolecular Interaction Geometries by a Hybrid Raman-Infrared Multidimensional Coherent Spectroscopy: Implications for High Throughput Biology. , 2010, , .		0
98	Optical Proteomics Combining Nonlinear Electrokinetics and Coherent Two-Dimensional Infrared Spectroscopy. Biophysical Journal, 2010, 98, 17a.	0.5	0
99	Probing Synaptic Amyloid-Beta Aggregation Promoted by Copper Release. Biophysical Journal, 2018, 114, 430a.	0.5	0
100	Parameters controlling electron injection kinetics in ruthenium bipyridyl dye sensitised titanium dioxide nanocrystalline films. , 2000, , .		0
101	Photoselective Excitation of P680 ?. , 1995, , 607-610.		0
102	Comparison of PS II Primary Photochemistry in Higher Plant, Synechocystis and Synechocystis Mutants. , 1995, , 615-618.		0
103	The Effect of Temperature on P680+ Reduction Kinetics During Water Splitting. , 1998, , 1045-1048.		0