Gary W Brudvig

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

255 papers	19,273 citations	73 h-index	133 g-index
276 ext. papers	21,270 ext. citations	10.1 avg, IF	7.05 L-index

#	Paper	IF	Citations
255	Optimization of Surface Loading of the Silatrane Anchoring Group on TiO.. *ACS Applied Materials & Interfaces*, **2022**,	9.5	2
254	Comparison of PsbQ and Psb27 in photosystem II provides insight into their roles.. *Photosynthesis Research*, **2022**, 1	3.7	1
253	High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, sp. PCC 6803.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119,	11.5	7
252	Glycerol binding at the narrow channel of photosystem II stabilizes the low-spin S state of the oxygen-evolving complex.. *Photosynthesis Research*, **2022**, 1	3.7	
251	Structure of a monomeric photosystem II core complex from a cyanobacterium acclimated to far-red light reveals the functions of chlorophylls d and f. *Journal of Biological Chemistry*, **2021**, 101424	5.4	6
250	Structure of a photosystem I-ferredoxin complex from a marine cyanobacterium provides insights into far-red light photoacclimation. *Journal of Biological Chemistry*, **2021**, 101408	5.4	2
249	Heterogeneous Composition of Oxygen-Evolving Complexes in Crystal Structures of Dark-Adapted Photosystem II. *Biochemistry*, **2021**, 60, 3374-3384	3.2	2
248	Nanotechnology for catalysis and solar energy conversion. *Nanotechnology*, **2021**, 32, 042003	3.4	24
247	Tuning the Conduction Band for Interfacial Electron Transfer: Dye-Sensitized SnxTi1⊠O2 Photoanodes for Water Splitting. *ACS Applied Energy Materials*, **2021**, 4, 4695-4703	6.1	2
246	Is Deprotonation of the Oxygen-Evolving Complex of Photosystem II during the S -jS Transition Suppressed by Proton Quantum Delocalization?. *Journal of the American Chemical Society*, **2021**, 143, 8324-8332	16.4	7
245	Experimental Verification of Ir 5d Orbital States and Atomic Structures in Highly Active Amorphous Iridium Oxide Catalysts. *ACS Catalysis*, **2021**, 11, 10084-10094	13.1	1
244	Cation-exchanged conductive Mn2DSBDC metal□rganic frameworks: Synthesis, structure, and THz conductivity. *Polyhedron*, **2021**, 203, 115182	2.7	2
243	Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light. *BBA Advances*, **2021**, 1, 100019		3
242	Kinetic modeling of substrate-water exchange in Photosystem II. *BBA Advances*, **2021**, 1, 100014		1
241	Proton exit pathways surrounding the oxygen evolving complex of photosystem II. *Biochimica Et Biophysica Acta - Bioenergetics*, **2021**, 1862, 148446	4.6	5
240	Observation of a potential-dependent switch of water-oxidation mechanism on Co-oxide-based catalysts. *CheM*, **2021**, 7, 2101-2117	16.2	11
239	Distorted Copper(II) Complex with Unusually Short CF⊠Cu Distances. *Inorganic Chemistry*, **2021**, 60, 14759-14764	5.1	4

238	Accessing Molecular Dimeric Ir Water Oxidation Catalysts from Coordination Precursors. *Inorganic Chemistry*, **2021**, 60, 14349-14356	5.1	2
237	Organometallic complexes as preferred precursors to form molecular Ir(pyalk) coordination complexes for catalysis of oxygen evolution. *Inorganica Chimica Acta*, **2021**, 526, 120507	2.7	1
236	Toward understanding the S2-S3 transition in the Kok cycle of Photosystem II: Lessons from Sr-substituted structure. *Inorganic Chemistry Communication*, **2021**, 133, 108890	3.1	3
235	Ultrafast terahertz spectroscopy provides insight into charge transfer efficiency and dynamics in artificial photosynthesis. *Photosynthesis Research*, **2020**, 1	3.7	0
234	Surprisingly big linker-dependence of activity and selectivity in CO reduction by an iridium(i) pincer complex. *Chemical Communications*, **2020**, 56, 9126-9129	5.8	6
233	Identification of a Na-Binding Site near the Oxygen-Evolving Complex of Spinach Photosystem II. *Biochemistry*, **2020**, 59, 2823-2831	3.2	2
232	Tribute to Charles A. Schmuttenmaer. *Journal of Physical Chemistry C*, **2020**, 124, 22333-22334	3.8	
231	Concerted proton-electron transfer oxidation of phenols and hydrocarbons by a high-valent nickel complex. *Chemical Science*, **2020**, 11, 1683-1690	9.4	9
230	Heterogeneous Nature of Electrocatalytic CO/CO Reduction by Cobalt Phthalocyanines. *ChemSusChem*, **2020**, 13, 6296-6299	8.3	8
229	Diazo coupling for surface attachment of small molecules to TiO nanoparticles. *Chemical Communications*, **2020**, 56, 9340-9343	5.8	4
228	D1-S169A substitution of photosystem II reveals a novel S-state structure. *Biochimica Et Biophysica Acta - Bioenergetics*, **2020**, 1861, 148301	4.6	3
227	Cryo-EM Structure of Monomeric Photosystem II from Synechocystis sp. PCC 6803 Lacking the Water-Oxidation Complex. *Joule*, **2020**, 4, 2131-2148	27.8	22
226	Opportunities and challenges for assigning cofactors in cryo-EM density maps of chlorophyll-containing proteins. *Communications Biology*, **2020**, 3, 408	6.7	11
225	Surface-Attached Molecular Catalysts on Visible-Light-Absorbing Semiconductors: Opportunities and Challenges for a Stable Hybrid Water-Splitting Photoanode. *ACS Energy Letters*, **2020**, 5, 3195-3202	20.1	12
224	Bis(dialkylphosphino)ferrocene-Ligated Nickel(II) Precatalysts for Suzuki-Miyaura Reactions of Aryl Carbonates. *Organometallics*, **2019**, 38, 3377-3387	3.8	15
223	Thermodynamics of the S-to-S state transition of the oxygen-evolving complex of photosystem II. *Physical Chemistry Chemical Physics*, **2019**, 21, 20840-20848	3.6	12
222	Insights into Proton-Transfer Pathways during Water Oxidation in Photosystem II. *Journal of Physical Chemistry B*, **2019**, 123, 8195-8202	3.4	11
221	Strongly Coupled Phenazine-Porphyrin Dyads: Light-Harvesting Molecular Assemblies with Broad Absorption Coverage. *ACS Applied Materials & Interfaces*, **2019**, 11, 8000-8008	9.5	28

220	D1-S169A Substitution of Photosystem II Perturbs Water Oxidation. *Biochemistry*, **2019**, 58, 1379-1387	3.2	15
219	Bicarbonate rescues damaged proton-transfer pathway in photosystem II. *Biochimica Et Biophysica Acta - Bioenergetics*, **2019**, 1860, 611-617	4.6	4
218	Metal-Organic Framework Photoconductivity via Time-Resolved Terahertz Spectroscopy. *Journal of the American Chemical Society*, **2019**, 141, 9793-9797	16.4	22
217	Synthesis and Reactivity of Paramagnetic Nickel Polypyridyl Complexes Relevant to C(sp)-C(sp)Coupling Reactions. *Angewandte Chemie - International Edition*, **2019**, 58, 6094-6098	16.4	44
216	Development of an Improved System for the Carboxylation of Aryl Halides through Mechanistic Studies. *ACS Catalysis*, **2019**, 9, 3228-3241	13.1	52
215	Collaboration between experiment and theory in solar fuels research. *Chemical Society Reviews*, **2019**, 48, 1865-1873	58.5	11
214	Synthesis and Reactivity of Paramagnetic Nickel Polypyridyl Complexes Relevant to C(sp2)C(sp3)Coupling Reactions. *Angewandte Chemie*, **2019**, 131, 6155-6159	3.6	4
213	Relative stability of the S isomers of the oxygen evolving complex of photosystem II. *Photosynthesis Research*, **2019**, 141, 331-341	3.7	12
212	Silatrane Anchors for Metal Oxide Surfaces: Optimization for Potential Photocatalytic and Electrocatalytic Applications. *ACS Applied Materials & Interfaces*, **2019**, 11, 5602-5609	9.5	21
211	Facet-Dependent Kinetics and Energetics of Hematite for Solar Water Oxidation Reactions. *ACS Applied Materials & Interfaces*, **2019**, 11, 5616-5622	9.5	32
210	Progress Towards Unraveling the Water-Oxidation Mechanism of Photosystem II **2019**, 285-306		
209	Light-Driven Water Oxidation with the Catalyst and the Ru(bpy)/SO Cycle: Photogeneration of Active Dimers, Electron-Transfer Kinetics, and Light Synchronization for Oxygen Evolution with High Quantum Efficiency. *Inorganic Chemistry*, **2019**, 58, 16537-16545	5.1	7
208	Modification of a pyridine-alkoxide ligand during the synthesis of coordination compounds. *Inorganica Chimica Acta*, **2019**, 484, 75-78	2.7	
207	N,N,O Pincer Ligand with a Deprotonatable Site That Promotes Redox-Leveling, High Mn Oxidation States, and a Mn2O2 Dimer Competent for Catalytic Oxygen Evolution. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2115-2123	2.3	6
206	Highly Active NiO Photocathodes for HO Production Enabled via Outer-Sphere Electron Transfer. *Journal of the American Chemical Society*, **2018**, 140, 4079-4084	16.4	50
205	Stable iridium dinuclear heterogeneous catalysts supported on metal-oxide substrate for solar water oxidation. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2902-2907	11.5	156
204	Selective CO Production by Photoelectrochemical Methane Oxidation on TiO. *ACS Central Science*, **2018**, 4, 631-637	16.8	30
203	Oxidation of Organic Compounds in Water by Unactivated Peroxymonosulfate. *Environmental Science & Technology*, **2018**, 52, 5911-5919	10.3	306

202	A Dinuclear Iridium(V,V) Oxo-Bridged Complex Characterized Using a Bulk Electrolysis Technique for Crystallizing Highly Oxidizing Compounds. *Inorganic Chemistry*, **2018**, 57, 5684-5691	5.1	12
201	Direct Interfacial Electron Transfer from High-Potential Porphyrins into Semiconductor Surfaces: A Comparison of Linkers and Anchoring Groups. *Journal of Physical Chemistry C*, **2018**, 122, 13529-13539	3.8	25
200	Nickel(I) Aryl Species: Synthesis, Properties, and Catalytic Activity. *ACS Catalysis*, **2018**, 8, 2526-2533	13.1	42
199	Endothelial Cell Autonomous Role of Akt1: Regulation of Vascular Tone and Ischemia-Induced Arteriogenesis. *Arteriosclerosis, Thrombosis, and Vascular Biology*, **2018**, 38, 870-879	9.4	26
198	Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. *Nature Communications*, **2018**, 9, 415	17.4	338
197	Substitution of the D1-Asn site in photosystem II of cyanobacteria mimics the chloride-binding characteristics of spinach photosystem II. *Journal of Biological Chemistry*, **2018**, 293, 2487-2497	5.4	20
196	End-On Bound Iridium Dinuclear Heterogeneous Catalysts on WO for Solar Water Oxidation. *ACS Central Science*, **2018**, 4, 1166-1172	16.8	54
195	Water-Nucleophilic Attack Mechanism for the CuII(pyalk)2 Water-Oxidation Catalyst. *ACS Catalysis*, **2018**, 8, 7952-7960	13.1	30
194	Reduced Occupancy of the Oxygen-Evolving Complex of Photosystem II Detected in Cryo-Electron Microscopy Maps. *Biochemistry*, **2018**, 57, 5925-5929	3.2	2
193	Modifications to the Aryl Group of dppf-Ligated Ni -Aryl Precatalysts: Impact on Speciation and Catalytic Activity in Suzuki-Miyaura Coupling Reactions. *Organometallics*, **2018**, 37, 3943-3955	3.8	15
192	Unusual Stability of a Bacteriochlorin Electrocatalyst under Reductive Conditions. A Case Study on CO2 Conversion to CO. *ACS Catalysis*, **2018**, 8, 10131-10136	13.1	21
191	Some crystal growth strategies for diffraction structure studies of iridium complexes. *Inorganica Chimica Acta*, **2018**, 480, 183-188	2.7	1
190	Energetics of the S State Spin Isomers of the Oxygen-Evolving Complex of Photosystem II. *Journal of Physical Chemistry B*, **2017**, 121, 1020-1025	3.4	31
189	Insights into Photosystem II from Isomorphous Difference Fourier Maps of Femtosecond X-ray Diffraction Data and Quantum Mechanics/Molecular Mechanics Structural Models. *ACS Energy Letters*, **2017**, 2, 397-407	20.1	15
188	Photodriven Oxidation of Surface-Bound Iridium-Based Molecular Water-Oxidation Catalysts on Perylene-3,4-dicarboximide-Sensitized TiO2 Electrodes Protected by an Al2O3 Layer. *Journal of Physical Chemistry C*, **2017**, 121, 3752-3764	3.8	35
187	Progress Toward a Molecular Mechanism of Water Oxidation in Photosystem II. *Annual Review of Physical Chemistry*, **2017**, 68, 101-116	15.7	111
186	A Pyridine Alkoxide Chelate Ligand That Promotes Both Unusually High Oxidation States and Water-Oxidation Catalysis. *Accounts of Chemical Research*, **2017**, 50, 952-959	24.3	63
185	Slow Equilibration between Spectroscopically Distinct Trap States in Reduced TiO Nanoparticles. *Journal of the American Chemical Society*, **2017**, 139, 2868-2871	16.4	20

184	A pomegranate-structured sulfur cathode material with triple confinement of lithium polysulfides for high-performance lithium–sulfur batteries. *Journal of Materials Chemistry A*, **2017**, 5, 11788-11793	13	18
183	Antimony Complexes for Electrocatalysis: Activity of a Main-Group Element in Proton Reduction. *Angewandte Chemie - International Edition*, **2017**, 56, 9111-9115	16.4	28
182	Anchoring groups for photocatalytic water oxidation on metal oxide surfaces. *Chemical Society Reviews*, **2017**, 46, 6099-6110	58.5	146
181	Synthesis of pyridine-alkoxide ligands for formation of polynuclear complexes. *New Journal of Chemistry*, **2017**, 41, 6709-6719	3.6	9
180	Electrocatalytic Water Oxidation by a Copper(II) Complex of an Oxidation-Resistant Ligand. *ACS Catalysis*, **2017**, 7, 3384-3387	13.1	109
179	Ultrathin dendrimer-graphene oxide composite film for stable cycling lithium-sulfur batteries. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 3578-3583	11.5	78
178	Solvent Dependence of Lateral Charge Transfer in a Porphyrin Monolayer. *ACS Energy Letters*, **2017**, 2, 168-173	20.1	11
177	Mechanistic Study of an Improved Ni Precatalyst for Suzuki-Miyaura Reactions of Aryl Sulfamates: Understanding the Role of Ni(I) Species. *Journal of the American Chemical Society*, **2017**, 139, 922-936	16.4	102
176	The O-Evolving Complex of Photosystem II: Recent Insights from Quantum Mechanics/Molecular Mechanics (QM/MM), Extended X-ray Absorption Fine Structure (EXAFS), and Femtosecond X-ray Crystallography Data. *Accounts of Chemical Research*, **2017**, 50, 41-48	24.3	134
175	On the relationship between cumulative correlation coefficients and the quality of crystallographic data sets. *Protein Science*, **2017**, 26, 2410-2416	6.3	3
174	X-ray Free Electron Laser Radiation Damage through the S-State Cycle of the Oxygen-Evolving Complex of Photosystem II. *Journal of Physical Chemistry B*, **2017**, 121, 9382-9388	3.4	13
173	Stereodynamic Quinone-Hydroquinone Molecules That Enantiomerize at sp-Carbon via Redox-Interconversion. *Journal of the American Chemical Society*, **2017**, 139, 15239-15244	16.4	13
172	Crystallographic Data Support the Carousel Mechanism of Water Supply to the Oxygen-Evolving Complex of Photosystem II. *ACS Energy Letters*, **2017**, 2, 2299-2306	20.1	43
171	Linker Length-Dependent Electron-Injection Dynamics of Trimesitylporphyrins on SnO2 Films. *Journal of Physical Chemistry C*, **2017**, 121, 22690-22699	3.8	10
170	Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,O-Donor Organic Ligand. *Angewandte Chemie*, **2017**, 129, 13227-13231	3.6	7
169	Optimization of Photoanodes for Photocatalytic Water Oxidation by Combining a Heterogenized Iridium Water-Oxidation Catalyst with a High-Potential Porphyrin Photosensitizer. *ChemSusChem*, **2017**, 10, 4526-4534	8.3	25
168	Electroreduction of CO Catalyzed by a Heterogenized Zn-Porphyrin Complex with a Redox-Innocent Metal Center. *ACS Central Science*, **2017**, 3, 847-852	16.8	130
167	Antimony Complexes for Electrocatalysis: Activity of a Main-Group Element in Proton Reduction. *Angewandte Chemie*, **2017**, 129, 9239-9243	3.6	6

166	Chlorophyll a with a farnesyl tail in thermophilic cyanobacteria. *Photosynthesis Research*, **2017**, 134, 175-182	3.7	12
165	Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,O-Donor Organic Ligand. *Angewandte Chemie - International Edition*, **2017**, 56, 13047-13051	16.4	15
164	Characterization of ammonia binding to the second coordination shell of the oxygen-evolving complex of photosystem II. *Dalton Transactions*, **2017**, 46, 16089-16095	4.3	7
163	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. *Journal of the American Chemical Society*, **2017**, 139, 9672-9683	16.4	34
162	A full set of iridium(iv) pyridine-alkoxide stereoisomers: highly geometry-dependent redox properties. *Chemical Science*, **2017**, 8, 1642-1652	9.4	27
161	Catalytic Oxygen Evolution from Manganese Complexes with an Oxidation-Resistant N,N,O-Donor Ligand. *ChemPlusChem*, **2016**, 81, 1129-1132	2.8	10
160	Controlling the rectification properties of molecular junctions through molecule-electrode coupling. *Nanoscale*, **2016**, 8, 16357-16362	7.7	28
159	Rutile TiO2 as an Anode Material for Water-Splitting Dye-Sensitized Photoelectrochemical Cells. *ACS Energy Letters*, **2016**, 1, 603-606	20.1	51
158	Ammonia Binding in the Second Coordination Sphere of the Oxygen-Evolving Complex of Photosystem II. *Biochemistry*, **2016**, 55, 4432-6	3.2	12
157	High Oxidation State Iridium Mono-μ-oxo Dimers Related to Water Oxidation Catalysis. *Journal of the American Chemical Society*, **2016**, 138, 15917-15926	16.4	31
156	Ferrocene-Promoted Long-Cycle Lithium–Sulfur Batteries. *Angewandte Chemie*, **2016**, 128, 15038-15042	3.6	11
155	Ferrocene-Promoted Long-Cycle Lithium-Sulfur Batteries. *Angewandte Chemie - International Edition*, **2016**, 55, 14818-14822	16.4	34
154	Heme biomolecule as redox mediator and oxygen shuttle for efficient charging of lithium-oxygen batteries. *Nature Communications*, **2016**, 7, 12925	17.4	98
153	A [3Fe-4S] cluster is required for tRNA thiolation in archaea and eukaryotes. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12703-12708	11.5	48
152	Electrochemical CO2 Reduction to Hydrocarbons on a Heterogeneous Molecular Cu Catalyst in Aqueous Solution. *Journal of the American Chemical Society*, **2016**, 138, 8076-9	16.4	329
151	Surface-Induced Deprotection of THP-Protected Hydroxamic Acids on Titanium Dioxide. *Journal of Physical Chemistry C*, **2016**, 120, 12495-12502	3.8	9
150	Molecular design of light-harvesting photosensitizers: effect of varied linker conjugation on interfacial electron transfer. *Physical Chemistry Chemical Physics*, **2016**, 18, 18678-82	3.6	17
149	Structure–function relationships in single molecule rectification by N-phenylbenzamide derivatives. *New Journal of Chemistry*, **2016**, 40, 7373-7378	3.6	6

148	New Ir Bis-Carbonyl Precursor for Water Oxidation Catalysis. *Inorganic Chemistry*, **2016**, 55, 2427-35	5.1	26
147	S3 State of the O2-Evolving Complex of Photosystem II: Insights from QM/MM, EXAFS, and Femtosecond X-ray Diffraction. *Biochemistry*, **2016**, 55, 981-4	3.2	51
146	Molecular titanium-hydroxamate complexes as models for TiO2 surface binding. *Chemical Communications*, **2016**, 52, 2972-5	5.8	21
145	Uncoupling Caveolae From Intracellular Signaling In Vivo. *Circulation Research*, **2016**, 118, 48-55	15.7	19
144	Heterogenized Iridium Water-Oxidation Catalyst from a Silatrane Precursor. *ACS Catalysis*, **2016**, 6, 5371-5377	13	63
143	High-Potential Porphyrins Supported on SnO2 and TiO2 Surfaces for Photoelectrochemical Applications. *Journal of Physical Chemistry C*, **2016**, 120, 28971-28982	3.8	21
142	Comparison of heterogenized molecular and heterogeneous oxide catalysts for photoelectrochemical water oxidation. *Energy and Environmental Science*, **2016**, 9, 1794-1802	35.4	104
141	Effect of Chloride Depletion on the Magnetic Properties and the Redox Leveling of the Oxygen-Evolving Complex in Photosystem II. *Journal of Physical Chemistry B*, **2016**, 120, 4243-8	3.4	20
140	Solution Structures of Highly Active Molecular Ir Water-Oxidation Catalysts from Density Functional Theory Combined with High-Energy X-ray Scattering and EXAFS Spectroscopy. *Journal of the American Chemical Society*, **2016**, 138, 5511-4	16.4	54
139	One-Step Trimethylstannylation of Benzyl and Alkyl Halides. *Journal of Organic Chemistry*, **2016**, 81, 9483-9488	4.7	1
138	Towards a Bioinspired-Systems Approach for Solar Fuel Devices. *ChemPlusChem*, **2016**, 81, 1024-1027	2.8	17
137	A molecular catalyst for water oxidation that binds to metal oxide surfaces. *Nature Communications* , **2015**, 6, 6469	17.4	218
136	Molecular Catalysts for Water Oxidation. *Chemical Reviews*, **2015**, 115, 12974-3005	68.1	787
135	Photoelectrochemical Cells Utilizing Tunable Corroles. *ACS Applied Materials & Interfaces*, **2015** , 7, 16124-30	9.5	33
134	Experimental Support for a Single Electron-Transfer Oxidation Mechanism in Firefly Bioluminescence. *Journal of the American Chemical Society*, **2015**, 137, 7592-5	16.4	61
133	Cation Effects on the Electron-Acceptor Side of Photosystem II. *Journal of Physical Chemistry B*, **2015**, 119, 7722-8	3.4	15
132	Stable Iridium(IV) Complexes of an Oxidation-Resistant Pyridine-Alkoxide Ligand: Highly Divergent Redox Properties Depending on the Isomeric Form Adopted. *Journal of the American Chemical Society*, **2015**, 137, 7243-50	16.4	41
131	Interfacial electron transfer in photoanodes based on phosphorus(V) porphyrin sensitizers co-deposited on SnO2 with the Ir(III)Cp* water oxidation precatalyst. *Journal of Materials Chemistry A*, **2015**, 3, 3868-3879	13	35

130	Iridium-based complexes for water oxidation. *Dalton Transactions*, **2015**, 44, 12452-72	4.3	133
129	NH3 Binding to the S2 State of the O2-Evolving Complex of Photosystem II: Analogue to H2O Binding during the S2 -jS3 Transition. *Biochemistry*, **2015**, 54, 5783-6	3.2	60
128	Preparation of Halogenated Fluorescent Diaminophenazine Building Blocks. *Journal of Organic Chemistry*, **2015**, 80, 9881-8	4.2	9
127	Computational Design of Intrinsic Molecular Rectifiers Based on Asymmetric Functionalization of N-Phenylbenzamide. *Journal of Chemical Theory and Computation*, **2015**, 11, 5888-96	6.4	29
126	Mechanism of Manganese-Catalyzed Oxygen Evolution from Experimental and Theoretical Analyses of 18O Kinetic Isotope Effects. *ACS Catalysis*, **2015**, 5, 7104-7113	13.1	35
125	Silatranes for binding inorganic complexes to metal oxide surfaces. *Dalton Transactions*, **2015**, 44, 20312-53	4.3	46
124	Comparison of dppf-Supported Nickel Precatalysts for the Suzuki–Miyaura Reaction: The Observation and Activity of Nickel(I). *Angewandte Chemie*, **2015**, 127, 13550-13554	3.6	15
123	Comparison of dppf-Supported Nickel Precatalysts for the Suzuki-Miyaura Reaction: The Observation and Activity of Nickel(I). *Angewandte Chemie - International Edition*, **2015**, 54, 13352-6	16.4	70
122	Hematite-Based Solar Water Splitting in Acidic Solutions: Functionalization by Mono- and Multilayers of Iridium Oxygen-Evolution Catalysts. *Angewandte Chemie - International Edition*, **2015**, 54, 11428-32	16.4	111
121	Photosynthetic water oxidation: binding and activation of substrate waters for O-O bond formation. *Faraday Discussions*, **2015**, 185, 37-50	3.6	56
120	Analysis of the radiation-damage-free X-ray structure of photosystem II in light of EXAFS and QM/MM data. *Biochemistry*, **2015**, 54, 1713-6	3.2	65
119	Photosynthetic water oxidation: insights from manganese model chemistry. *Accounts of Chemical Research*, **2015**, 48, 567-74	24.3	115
118	Towards multielectron photocatalysis: a porphyrin array for lateral hole transfer and capture on a metal oxide surface. *Physical Chemistry Chemical Physics*, **2015**, 17, 12728-34	3.6	24
117	A Stable Coordination Complex of Rh(IV) in an N,O-Donor Environment. *Journal of the American Chemical Society*, **2015**, 137, 15692-5	16.4	24
116	Facet-dependent photoelectrochemical performance of TiO2 nanostructures: an experimental and computational study. *Journal of the American Chemical Society*, **2015**, 137, 1520-9	16.4	205
115	Oxygen-evolving complex of Photosystem II: an analysis of second-shell residues and hydrogen-bonding networks. *Current Opinion in Chemical Biology*, **2015**, 25, 152-8	9.7	82
114	Probing the effect of mutations of asparagine 181 in the D1 subunit of photosystem II. *Biochemistry* , **2015**, 54, 1663-72	3.2	23
113	Computational insights on crystal structures of the oxygen-evolving complex of photosystem II with either Ca(2+) or Ca(2+) substituted by Sr(2+). *Biochemistry*, **2015**, 54, 820-5	3.2	28

112	Proton-Coupled Electron Transfer During the S-State Transitions of the Oxygen-Evolving Complex of Photosystem II. *Journal of Physical Chemistry B*, **2015**, 119, 7366-77	3.4	39
111	Insights into substrate binding to the oxygen-evolving complex of photosystem II from ammonia inhibition studies. *Biochemistry*, **2015**, 54, 622-8	3.2	22
110	Nickel(I) monomers and dimers with cyclopentadienyl and indenyl ligands. *Chemistry - A European Journal*, **2014**, 20, 5327-37	4.8	57
109	Organosilatrane building blocks. *Tetrahedron Letters*, **2014**, 55, 1062-1064	2	24
108	Photoelectrochemical hole injection revealed in polyoxotitanate nanocrystals functionalized with organic adsorbates. *Journal of the American Chemical Society*, **2014**, 136, 16420-9	16.4	59
107	Linker rectifiers for covalent attachment of transition-metal catalysts to metal-oxide surfaces. *ChemPhysChem*, **2014**, 15, 1138-47	3.2	18
106	Structural changes in the oxygen-evolving complex of photosystem II induced by the S1 to S2 transition: A combined XRD and QM/MM study. *Biochemistry*, **2014**, 53, 6860-2	3.2	39
105	Co(II), a catalyst for selective conversion of phenyl rings to carboxylic acid groups. *RSC Advances*, **2014**, 4, 49395-49399	3.7	4
104	Oxygen-evolving complex of photosystem II: correlating structure with spectroscopy. *Physical Chemistry Chemical Physics*, **2014**, 16, 11812-21	3.6	59
103	Electrochemical activation of Cp* iridium complexes for electrode-driven water-oxidation catalysis. *Journal of the American Chemical Society*, **2014**, 136, 13826-34	16.4	98
102	Structural Studies of Oxomanganese Complexes for Water Oxidation Catalysis **2014**, 1-14		
101	Modular Assembly of High-Potential Zinc Porphyrin Photosensitizers Attached to TiO2 with a Series of Anchoring Groups. *Journal of Physical Chemistry C*, **2013**, 117, 14526-14533	3.8	82
100	Probing the Viability of Oxo-Coupling Pathways in Iridium-Catalyzed Oxygen Evolution. *Organometallics*, **2013**, 32, 5384-5390	3.8	40
99	S0-State model of the oxygen-evolving complex of photosystem II. *Biochemistry*, **2013**, 52, 7703-6	3.2	84
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