Dimitrios A Pantazis

List of Publications by Year
in descending order

126 papers	9,433 citations	46918 47 h-index	40881 93 g-index
134 all docs	134 docs citations	134 times ranked	6900 citing authors

#	Article	IF	Citations
1	All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. Journal of Chemical Theory and Computation, 2008, 4, 908-919.	2.3	1,061
2	Biological Water Oxidation. Accounts of Chemical Research, 2013, 46, 1588-1596.	7.6	453
3	Electronic structure of the oxygen-evolving complex in photosystem II prior to O-O bond formation. Science, 2014, 345, 804-808.	6.0	432
4	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2008, 4, 1449-1459.	2.3	421
5	Two Interconvertible Structures that Explain the Spectroscopic Properties of the Oxygenâ€Evolving Complex of Photosystemâ€...II in the S₂ State. Angewandte Chemie - International Edition, 2012, 51, 9935-9940.	7.2	342
6	What is not required to make a single molecule magnet. Faraday Discussions, 2011, 148, 229-238.	1.6	313
7	All-Electron Scalar Relativistic Basis Sets for the Lanthanides. Journal of Chemical Theory and Computation, 2009, 5, 2229-2238.	2.3	293
8	Density functional theory. Photosynthesis Research, 2009, 102, 443-453.	1.6	282
9	Metal oxidation states in biological water splitting. Chemical Science, 2015, 6, 1676-1695.	3.7	275
10	Theoretical Evaluation of Structural Models of the S₂ State in the Oxygen Evolving Complex of Photosystem II: Protonation States and Magnetic Interactions. Journal of the American Chemical Society, 2011, 133, 19743-19757.	6.6	271
11	All-Electron Scalar Relativistic Basis Sets for the Actinides. Journal of Chemical Theory and Computation, 2011, 7, 677-684.	2.3	260
12	Effect of Ca²⁺/Sr²⁺ Substitution on the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II: A Combined Multifrequency EPR, ⁵⁵Mn-ENDOR, and DFT Study of the S₂ State. Journal of the American Chemical Society, 2011, 133, 3635-3648.	6.6	211
13	A five-coordinate Mn(<scp>iv</scp>) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. Chemical Science, 2016, 7, 72-84.	3.7	158
14	Experimental and Theoretical Investigations of New Dinuclear Palladium Complexes as Precatalysts for the Amination of Aryl Chlorides. Journal of the American Chemical Society, 2006, 128, 6376-6390.	6.6	148
15	Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (Ì¼-oxo) of the manganese tetramer. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15561-15566.	3.3	148
16	Detailed Ab Initio First-Principles Study of the Magnetic Anisotropy in a Family of Trigonal Pyramidal Iron(II) Pyrrolide Complexes. Inorganic Chemistry, 2011, 50, 7460-7477.	1.9	142
17	Missing Pieces in the Puzzle of Biological Water Oxidation. ACS Catalysis, 2018, 8, 9477-9507.	5.5	138
18	A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transitionâ€Metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystemâ€...II. Chemistry - A European Journal, 2009, 15, 5108-5123.	1.7	123

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19	Current Understanding of the Mechanism of Water Oxidation in Photosystem II and Its Relation to XFEL Data. Annual Review of Biochemistry, 2020, 89, 795-820.	5.0	123
20	Structure of the oxygen-evolving complex of photosystem II: information on the S2 state through quantum chemical calculation of its magnetic properties. Physical Chemistry Chemical Physics, 2009, 11, 6788.	1.3	121
21	All-electron scalar relativistic basis sets for the 6p elements. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	117
22	Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. Journal of Chemical Theory and Computation, 2016, 12, 1148-1156.	2.3	112
23	Magnetic and Spectroscopic Properties of Mixed Valence Manganese(III,IV) Dimers: A Systematic Study Using Broken Symmetry Density Functional Theory. Inorganic Chemistry, 2009, 48, 7251-7260.	1.9	107
24	<scp>Allâ€electron</scp> scalar relativistic basis sets for the elements Rbâ€“Xe. Journal of Computational Chemistry, 2020, 41, 1842-1849.	1.5	106
25	Theoretical magnetochemistry of dinuclear manganese complexes: broken symmetry density functional theory investigation on the influence of bridging motifs on structure and magnetism. Dalton Transactions, 2010, 39, 4959.	1.6	100
26	Recent developments in biological water oxidation. Current Opinion in Chemical Biology, 2016, 31, 113-119.	2.8	97
27	Ionization Energies and Aqueous Redox Potentials of Organic Molecules: Comparison of DFT, Correlated ab Initio Theory and Pair Natural Orbital Approaches. Journal of Chemical Theory and Computation, 2016, 12, 2272-2284.	2.3	94
28	On the Magnetic and Spectroscopic Properties of High-Valent Mn₃CaO₄ Cubanes as Structural Units of Natural and Artificial Water-Oxidizing Catalysts. Journal of the American Chemical Society, 2013, 135, 5726-5739.	6.6	88
29	Spin State as a Marker for the Structural Evolution of Natureâ€™s Water-Splitting Catalyst. Inorganic Chemistry, 2016, 55, 488-501.	1.9	87
30	The electronic structures of the S2 states of the oxygen-evolving complexes of photosystem II in plants and cyanobacteria in the presence and absence of methanol. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 829-840.	0.5	81
31	Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S2 state: a combined EPR and DFT study. Physical Chemistry Chemical Physics, 2014, 16, 11877.	1.3	77
32	Structural models of the biological oxygen-evolving complex: achievements, insights, and challenges for biomimicry. Green Chemistry, 2017, 19, 2309-2325.	4.6	74
33	A Three-State Model for the Polymorphism in Linear Tricobalt Compounds. Journal of the American Chemical Society, 2006, 128, 4128-4135.	6.6	71
34	The first tyrosyl radical intermediate formed in the S2â€“S3 transition of photosystem II. Physical Chemistry Chemical Physics, 2014, 16, 11901.	1.3	68
35	Accurate Computation of the Absorption Spectrum of Chlorophyll a with Pair Natural Orbital Coupled Cluster Methods. Journal of Physical Chemistry B, 2020, 124, 8761-8771.	1.2	65
36	The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived Î¼-Hydroxo Bridge. Journal of the American Chemical Society, 2017, 139, 14412-14424.	6.6	63

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37	Exchange Coupling Interactions from the Density Matrix Renormalization Group and N-Electron Valence Perturbation Theory: Application to a Biomimetic Mixed-Valence Manganese Complex. Journal of Chemical Theory and Computation, 2018, 14, 166-179.	2.3	62
38	Artificial photosynthesis: understanding water splitting in nature. Interface Focus, 2015, 5, 20150009.	1.5	60
39	Dioxygen Activation and Catalytic Reduction to Hydrogen Peroxide by a Thiolate-Bridged Dimanganese(II) Complex with a Pendant Thiol. Journal of the American Chemical Society, 2015, 137, 8644-8653.	6.6	56
40	Isolation and reactivity of an elusive diazoalkene. Nature Chemistry, 2021, 13, 587-593.	6.6	55
41	A Highly Reactive Ruthenium Phosphido Complex Exhibiting Ruâ•P Ï€-Bonding. Organometallics, 2007, 26, 1473-1482.	1.1	54
42	On the Origin of Î±- and Î²-Agostic Distortions in Early-Transition-Metal Alkyl Complexes. Organometallics, 2008, 27, 1128-1134.	1.1	54
43	Convergence of QM/MM and Cluster Models for the Spectroscopic Properties of the Oxygen-Evolving Complex in Photosystem II. Journal of Chemical Theory and Computation, 2013, 9, 3832-3842.	2.3	54
44	Trinuclear Terpyridine Frustrated Spin System with a Mn^{IV}₃O₄ Core: Synthesis, Physical Characterization, and Quantum Chemical Modeling of Its Magnetic Properties. Inorganic Chemistry, 2009, 48, 10281-10288.	1.9	53
45	Critical Role of the Correlation Functional in DFT Descriptions of an Agostic Niobium Complex. Journal of Chemical Theory and Computation, 2007, 3, 1329-1336.	2.3	52
46	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. Journal of Chemical Theory and Computation, 2012, 8, 2630-2645.	2.3	52
47	Principles of Natural Photosynthesis. Topics in Current Chemistry, 2015, 371, 23-48.	4.0	51
48	Activation of a water molecule using a mononuclear Mn complex: from Mn-aquo, to Mn-hydroxo, to Mn-oxyl via charge compensation. Energy and Environmental Science, 2010, 3, 924.	15.6	50
49	Multireference Approaches to Spinâ€State Energetics of Transition Metal Complexes Utilizing the Density Matrix Renormalization Group. Advanced Theory and Simulations, 2019, 2, 1800201.	1.3	50
50	Interaction of methanol with the oxygen-evolving complex: atomistic models, channel identification, species dependence, and mechanistic implications. Chemical Science, 2016, 7, 6463-6476.	3.7	47
51	Protein Matrix Control of Reaction Center Excitation in Photosystem II. Journal of the American Chemical Society, 2020, 142, 18174-18190.	6.6	46
52	Allâ€electron basis sets for heavy elements. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 363-374.	6.2	45
53	What Can We Learn from a Biomimetic Model of Natureâ€™s Oxygen-Evolving Complex?. Inorganic Chemistry, 2017, 56, 3875-3888.	1.9	40
54	Câ•H Bond Activation of Benzene by Unsaturated Î·²-Cyclopropene and Î·²-Benzyne Complexes of Niobium. Journal of the American Chemical Society, 2010, 132, 14239-14250.	6.6	39

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55	Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues. Physical Chemistry Chemical Physics, 2016, 18, 10739-10750.	1.3	38
56	Meeting the Challenge of Magnetic Coupling in a Triply-Bridged Chromium Dimer: Complementary Broken-Symmetry Density Functional Theory and Multireference Density Matrix Renormalization Group Perspectives. Journal of Chemical Theory and Computation, 2019, 15, 938-948.	2.3	38
57	Structure and bonding in the isoelectronic series CnHnP5â^'n+: is phosphorus a carbon copy?. Dalton Transactions, 2004, , 2080-2086.	1.6	37
58	Electronic Structural Flexibility of Heterobimetallic Mn/Fe Cofactors: R2lox and R2c Proteins. Journal of the American Chemical Society, 2014, 136, 13399-13409.	6.6	37
59	Evidence for a SN2-Type Pathway for Phosphine Exchange in Phosphineâ€“Phosphenium Cations, [R2Pï£¿PRâ€²3]+. Chemistry - A European Journal, 2007, 13, 6967-6974.	1.7	36
60	Dealing with Complexity in Open-Shell Transition Metal Chemistry from a Theoretical Perspective: Reaction Pathways, Bonding, Spectroscopy, And Magnetic Properties. Advances in Inorganic Chemistry, 2010, 62, 301-349.	0.4	36
61	A Main-Group Analogue of Housene: The Subtle Influence of the Inert-Pair Effect in Group 15 Clusters. Angewandte Chemie - International Edition, 2006, 45, 6685-6689.	7.2	35
62	Cationic phosphorusâ€“carbonâ€“pnictogen cages isolobal to [C5R5]+. Chemical Communications, 2006, , 1375.	2.2	33
63	1,2-Diphosphinobenzene as a synthon for the 1,2,3-triphospha- and 2-arsa-1,3-diphosphaindenyl anions and a stable organo derivative of the P8 unit of Hittorfâ€™s phosphorus. Chemical Communications, 2008, , 856.	2.2	32
64	A First-Principles Approach to the Calculation of the on-Site Zero-Field Splitting in Polynuclear Transition Metal Complexes. Inorganic Chemistry, 2014, 53, 11785-11793.	1.9	32
65	Structureâ€“Spectroscopy Correlations for Intermediate Q of Soluble Methane Monooxygenase: Insights from QM/MM Calculations. Journal of the American Chemical Society, 2021, 143, 6560-6577.	6.6	32
66	Differences in the Active Site of Water Oxidation among Photosynthetic Organisms. Journal of the American Chemical Society, 2017, 139, 14340-14343.	6.6	31
67	Orientational Jahnâ€“Teller Isomerism in the Darkâ€Stable State of Nature's Water Oxidase. Angewandte Chemie - International Edition, 2021, 60, 13493-13499.	7.2	29
68	The S3 State of the Oxygen-Evolving Complex: Overview of Spectroscopy and XFEL Crystallography with a Critical Evaluation of Early-Onset Models for Oâ€“O Bond Formation. Inorganics, 2019, 7, 55.	1.2	28
69	Proton Translocation via Tautomerization of Asn298 During the S₂â€“S₃ State Transition in the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2019, 123, 3068-3078.	1.2	28
70	Accurate computed spin-state energetics for Co(<scp>iii</scp>) complexes: implications for modelling homogeneous catalysis. Dalton Transactions, 2020, 49, 6478-6487.	1.6	28
71	Arrested Substrate Binding Resolves Catalytic Intermediates in Higherâ€Plant Water Oxidation. Angewandte Chemie - International Edition, 2021, 60, 3156-3162.	7.2	28
72	Characterization of Oxygen Bridged Manganese Model Complexes Using Multifrequency ¹⁷O-Hyperfine EPR Spectroscopies and Density Functional Theory. Journal of Physical Chemistry B, 2015, 119, 13904-13921.	1.2	27

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73	Câ^'C Coupling Constants, JCC, Are Reliable Probes for Î±-Câ^'C Agostic Structures. Organometallics, 2009, 28, 940-943.	1.1	26
74	How Accurately Can Extended X-ray Absorption Spectra Be Predicted from First Principles? Implications for Modeling the Oxygen-Evolving Complex in Photosystem II. Journal of the American Chemical Society, 2015, 137, 12815-12834.	6.6	26
75	Resolving the Manganese Oxidation States in the Oxygenâ€evolving Catalyst of Natural Photosynthesis. Israel Journal of Chemistry, 2015, 55, 1219-1232.	1.0	25
76	Accurate Spin-State Energetics for Aryl Carbenes. Journal of Chemical Theory and Computation, 2018, 14, 4733-4746.	2.3	25
77	On the Nature of the Bonding in 1:1 Adducts of O2. Inorganic Chemistry, 2003, 42, 7734-7736.	1.9	24
78	Concerted [2+2]â€...Cycloaddition of Alkenes to a Rutheniumâ€“Phosphorus Double Bond. Angewandte Chemie - International Edition, 2010, 49, 3367-3370.	7.2	24
79	Implications of structural heterogeneity for the electronic structure of the final oxygen-evolving intermediate in photosystem II. Journal of Inorganic Biochemistry, 2019, 199, 110797.	1.5	24
80	Successes, challenges, and opportunities for quantum chemistry in understanding metalloenzymes for solar fuels research. Chemical Communications, 2021, 57, 3952-3974.	2.2	24
81	Benzonitrile Adducts of Terminal Diarylphosphido Complexes: Preparative Sources of â€œRuâ•PR₂â€• Organometallics, 2011, 30, 6458-6465.	1.1	23
82	Synthesis and Computational Studies of Palladium(I) Dimers Pd2X2(PtBu2Ph)2(X = Br, I):Â Phenyl versus Halide Bridging Modes. Organometallics, 2006, 25, 5990-5995.	1.1	22
83	A re-evaluation of the two-step spin crossover in the trinuclear cation [Co₃(dipyridylamido)₄Cl₂]⁺. Dalton Transactions, 2008, , 608-614.	1.6	22
84	A New Reaction Pathway in Organophosphorus Chemistry: Competing SN2 and AEâ€² Pathways for Nucleophilic Attack at a Phosphorusâ€“Carbon Cage Compound. Angewandte Chemie - International Edition, 2006, 45, 3628-3631.	7.2	21
85	Axial ligand effect on the catalytic activity of biomimetic Fe-porphyrin catalyst: An experimental and DFT study. Journal of Catalysis, 2016, 344, 768-777.	3.1	20
86	Redox Isomerism in the S₃ State of the Oxygenâ€Evolving Complex Resolved by Coupled Cluster Theory. Chemistry - A European Journal, 2021, 27, 12815-12825.	1.7	20
87	Reconciling Local Coupled Cluster with Multireference Approaches for Transition Metal Spin-State Energetics. Journal of Chemical Theory and Computation, 2022, 18, 3538-3548.	2.3	20
88	Assessment of Double-Hybrid Density Functional Theory for Magnetic Exchange Coupling in Manganese Complexes. Inorganics, 2019, 7, 57.	1.2	19
89	Physical Nature of Differential Spin-State Stabilization of Carbenes by Hydrogen and Halogen Bonding: A Domain-Based Pair Natural Orbital Coupled Cluster Study. Journal of Physical Chemistry A, 2019, 123, 5081-5090.	1.1	19
90	Performance of density functional theory and orbital-optimised second-order perturbation theory methods for geometries and singletâ€“triplet state splittings of aryl-carbenes. Molecular Physics, 2020, 118, e1764644.	0.8	19

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91	How Can We Predict Accurate Electrochromic Shifts for Biochromophores? A Case Study on the Photosynthetic Reaction Center. Journal of Chemical Theory and Computation, 2021, 17, 1858-1873.	2.3	18
92	Comparison of Density Functional and Correlated Wave Function Methods for the Prediction of Cu(II) Hyperfine Coupling Constants. ChemPhysChem, 2020, 21, 2667-2679.	1.0	16
93	Calcium and heterometallic manganeseâ€“calcium complexes supported by tripodal pyridine-carboxylate ligands: structural, EPR and theoretical investigations. Dalton Transactions, 2015, 44, 12757-12770.	1.6	15
94	Calcium Valence-to-Core X-ray Emission Spectroscopy: A Sensitive Probe of Oxo Protonation in Structural Models of the Oxygen-Evolving Complex. Inorganic Chemistry, 2019, 58, 16292-16301.	1.9	15
95	Understanding and tuning the properties of redox-accumulating manganese helicates. Dalton Transactions, 2016, 45, 18900-18908.	1.6	14
96	Orbital Entanglement Analysis of Exchange-Coupled Systems. Journal of Physical Chemistry Letters, 2019, 10, 6762-6770.	2.1	14
97	Microsolvation of the Redox-Active Tyrosine-D in Photosystem II: Correlation of Energetics with EPR Spectroscopy and Oxidation-Induced Proton Transfer. Journal of the American Chemical Society, 2019, 141, 3217-3231.	6.6	14
98	Spin-state energetics of manganese spin crossover complexes: Comparison of single-reference and multi-reference ab initio approaches. Polyhedron, 2021, 208, 115399.	1.0	14
99	Alkene Insertions into a Ruâ€“PR‹sub›2‹/sub› Bond. Organometallics, 2016, 35, 3970-3980.	1.1	13
100	Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	13
101	The Electronic Origin of Farâ€Redâ€Lightâ€Driven Oxygenic Photosynthesis. Angewandte Chemie - International Edition, 2022, 61, .	7.2	13
102	Crystalline Germanium(I) and Tin(I) Centered Radical Anions. Angewandte Chemie - International Edition, 2022, 61, .	7.2	13
103	Characterization of a Triplet Vinylidene. Journal of the American Chemical Society, 2021, 143, 21410-21415.	6.6	13
104	Theoretical Study on the Mechanism of Reaction of Ground-State Fe Atoms with Carbon Dioxide. Collection of Czechoslovak Chemical Communications, 2004, 69, 13-33.	1.0	12
105	Chlorophyll excitation energies and structural stability of the CP47 antenna of photosystem II: a case study in the first-principles simulation of light-harvesting complexes. Chemical Science, 2021, 12, 4463-4476.	3.7	11
106	Promotion of phosphaalkyne cyclooligomerisation by a Sb(v) to Sb(iii) redox process. Dalton Transactions, 2008, , 3753.	1.6	10
107	Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. Inorganic Chemistry, 2021, 60, 7399-7412.	1.9	10
108	Ab Initio Quantum Chemical Study of the Coordination Preferences and Catalytic Role of Cu+ Ions in the Dehydration Reactions of Hydroxyformaldoxime Conformers and the Oxidation of HCN to Hydroxyformaldoxime by Hydrogen Peroxide. Journal of Physical Chemistry A, 2002, 106, 1425-1440.	1.1	9

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109	Systematic Highâ€Accuracy Prediction of Electron Affinities for Biological Quinones. Journal of Computational Chemistry, 2018, 39, 2439-2451.	1.5	9
110	Ionization Energies and Redox Potentials of Hydrated Transition Metal Ions: Evaluation of Domain-Based Local Pair Natural Orbital Coupled Cluster Approaches. Journal of Chemical Theory and Computation, 2022, 18, 1619-1632.	2.3	9
111	Evaluation of new low-valent computational models for the oxygen-evolving complex of photosystem II. Chemical Physics Letters, 2020, 753, 137629.	1.2	8
112	Applications of the Density Matrix Renormalization Group to Exchange-Coupled Transition Metal Systems. Challenges and Advances in Computational Chemistry and Physics, 2019, , 91-120.	0.6	7
113	Unusual ³¹P Hyperfine Strain Effects in a Conformationally Flexible Cu(II) Complex Revealed by Two-Dimensional Pulse EPR Spectroscopy. Inorganic Chemistry, 2020, 59, 3666-3676.	1.9	7
114	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. Magnetochemistry, 2022, 8, 36.	1.0	7
115	First-Principles Calculation of Transition Metal Hyperfine Coupling Constants with the Strongly Constrained and Appropriately Normed (SCAN) Density Functional and its Hybrid Variants. Magnetochemistry, 2019, 5, 69.	1.0	6
116	Reversible Silylium Transfer between Pâ€H and Siâ€H Donors. Angewandte Chemie - International Edition, 2021, 60, 2379-2384.	7.2	5
117	The Reactivity of the Imine Bond within Polynuclear Nickel(II) Complexes. Crystals, 2021, 11, 512.	1.0	5
118	Arrested Substrate Binding Resolves Catalytic Intermediates in Higherâ€Plant Water Oxidation. Angewandte Chemie, 2021, 133, 3193-3199.	1.6	4
119	12 Biological water splitting. , 2021, , 427-468.		4
120	The Electronic Origin of Farâ€Redâ€Lightâ€Driven Oxygenic Photosynthesis. Angewandte Chemie, 2022, 134, .	1.6	4
121	Crystalline Germanium(I) and Tin(I) Centered Radical Anions. Angewandte Chemie, 2022, 134, .	1.6	4
122	Decoding the Ambiguous Electron Paramagnetic Resonance Signals in the Lytic Polysaccharide Monooxygenase from Photorhabdus luminescens. Inorganic Chemistry, 2022, 61, 8022-8035.	1.9	4
123	Orientational Jahnâ€“Teller Isomerism in the Darkâ€Stable State of Nature's Water Oxidase. Angewandte Chemie, 2021, 133, 13605-13611.	1.6	3
124	Reversible Silylium Transfer between Pâ€H and Siâ€H Donors. Angewandte Chemie, 2021, 133, 2409-2414.	1.6	2
125	Electronic properties of the SÂ=Â5/2 Mn(II) complexes [Mn{PhC(O)NP(O)PPh2}(N,N)(NO3)], (N,N)Â=Âphenanthroline, neocuproine, 2,2â€²-bipyridine. Polyhedron, 2021, 207, 115374.	1.0	2
126	Electrostatic profiling of photosynthetic pigments: implications for directed spectral tuning. Physical Chemistry Chemical Physics, 2021, 23, 24677-24684.	1.3	2