Dimitrios A Pantazis

List of Publications by Citations

124 papers	7,415 citations	43 h-index	84 g-index
134 ext. papers	8,386 ext. citations	7.8 avg, IF	6.59 L-index

#	Paper	IF	Citations
124	All-Electron Scalar Relativistic Basis Sets for Third-Row Transition Metal Atoms. *Journal of Chemical Theory and Computation*, **2008**, 4, 908-19	6.4	832
123	Biological water oxidation. *Accounts of Chemical Research*, **2013**, 46, 1588-96	24.3	407
122	Photosynthesis. Electronic structure of the oxygen-evolving complex in photosystem II prior to O-O bond formation. *Science*, **2014**, 345, 804-8	33.3	363
121	Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. *Journal of Chemical Theory and Computation*, **2008**, 4, 1449-59	6.4	363
120	Two interconvertible structures that explain the spectroscopic properties of the oxygen-evolving complex of photosystem II in the S2 state. *Angewandte Chemie - International Edition*, **2012**, 51, 9935-40	16.4	293
119	What is not required to make a single molecule magnet. *Faraday Discussions*, **2011**, 148, 229-38; discussion 299-314	3.6	265
118	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, 19743-57	16.4	249
117	All-Electron Scalar Relativistic Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2009**, 5, 2229-38	6.4	227
116	Metal oxidation states in biological water splitting. *Chemical Science*, **2015**, 6, 1676-1695	9.4	225
115	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, 3635-48	16.4	190
114	All-Electron Scalar Relativistic Basis Sets for the Actinides. *Journal of Chemical Theory and Computation*, **2011**, 7, 677-684	6.4	187
113	Density functional theory. *Photosynthesis Research*, **2009**, 102, 443-53	3.7	174
112	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, 6376-90	16.4	141
111	A five-coordinate Mn(iv) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. *Chemical Science*, **2016**, 7, 72-84	9.4	134
110	Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (Ebxo) of the manganese tetramer. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 15561-6	11.5	130
109	Detailed ab initio first-principles study of the magnetic anisotropy in a family of trigonal pyramidal iron(II) pyrrolide complexes. *Inorganic Chemistry*, **2011**, 50, 7460-77	5.1	120
108	Structure of the oxygen-evolving complex of photosystem II: information on the S(2) state through quantum chemical calculation of its magnetic properties. *Physical Chemistry Chemical Physics*, **2009**, 11, 6788-98	3.6	114

107	A new quantum chemical approach to the magnetic properties of oligonuclear transition-metal complexes: application to a model for the tetranuclear manganese cluster of photosystem II. *Chemistry - A European Journal*, **2009**, 15, 5108-23	4.8	106
106	Missing Pieces in the Puzzle of Biological Water Oxidation. *ACS Catalysis*, **2018**, 8, 9477-9507	13.1	101
105	Magnetic and spectroscopic properties of mixed valence manganese(III,IV) dimers: a systematic study using broken symmetry density functional theory. *Inorganic Chemistry*, **2009**, 48, 7251-60	5.1	98
104	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, 4959-67	4.3	93
103	Recent developments in biological water oxidation. *Current Opinion in Chemical Biology*, **2016**, 31, 113-9	9.7	87
102	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, 5726-39	16.4	81
101	All-electron scalar relativistic basis sets for the 6p elements. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	79
100	The electronic structures of the S(2) 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, 829-40	4.6	75
99	Spin State as a Marker for the Structural Evolution of Nature's Water-Splitting Catalyst. *Inorganic Chemistry*, **2016**, 55, 488-501	5.1	70
98	A three-state model for the polymorphism in linear tricobalt compounds. *Journal of the American Chemical Society*, **2006**, 128, 4128-35	16.4	68
97	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, 2272-84	6.4	68
96	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, 11877-92	3.6	66
95	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	29.1	62
94	Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. *Journal of Chemical Theory and Computation*, **2016**, 12, 1148-56	6.4	62
93	The first tyrosyl radical intermediate formed in the S2-S3 transition of photosystem II. *Physical Chemistry Chemical Physics*, **2014**, 16, 11901-10	3.6	60
92	Structural models of the biological oxygen-evolving complex: achievements, insights, and challenges for biomimicry. *Green Chemistry*, **2017**, 19, 2309-2325	10	55
91	On the Origin of □and □Agostic Distortions in Early-Transition-Metal Alkyl Complexes. *Organometallics*, **2008**, 27, 1128-1134	3.8	51
90	Critical Role of the Correlation Functional in DFT Descriptions of an Agostic Niobium Complex. *Journal of Chemical Theory and Computation*, **2007**, 3, 1329-36	6.4	51

89	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, 3832-42	6.4	50
88	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, 10281-8	5.1	50
87	The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived Hydroxo Bridge. *Journal of the American Chemical Society*, **2017**, 139, 14412-14424	16.4	49
86	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. *Journal of Chemical Theory and Computation*, **2012**, 8, 2630-45	6.4	49
85	Activation of a water molecule using a mononuclear Mn complex: from Mn-aquo, to Mn-hydroxo, to Mn-oxyl charge compensation. *Energy and Environmental Science*, **2010**, 3, 924-938	35.4	49
84	Artificial photosynthesis: understanding water splitting in nature. *Interface Focus*, **2015**, 5, 20150009	3.9	47
83	A Highly Reactive Ruthenium Phosphido Complex Exhibiting Ru P Bonding. *Organometallics*, **2007**, 26, 1473-1482	3.8	45
82	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, 8644-53	16.4	44
81	Principles of Natural Photosynthesis. *Topics in Current Chemistry*, **2016**, 371, 23-48		40
80	Interaction of methanol with the oxygen-evolving complex: atomistic models, channel identification, species dependence, and mechanistic implications. *Chemical Science*, **2016**, 7, 6463-6476	9.4	40
79	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	6.4	40
78	What Can We Learn from a Biomimetic Model of Nature's Oxygen-Evolving Complex?. *Inorganic Chemistry*, **2017**, 56, 3875-3888	5.1	35
77	C-H bond activation of benzene by unsaturated -cyclopropene and -benzyne complexes of niobium. *Journal of the American Chemical Society*, **2010**, 132, 14239-50	16.4	35
76	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	2.1	33
75	Evidence for a SN2-type pathway for phosphine exchange in phosphine-phosphenium cations, [R2P--PR'3]+. *Chemistry - A European Journal*, **2007**, 13, 6967-74	4.8	33
74	Electronic structural flexibility of heterobimetallic Mn/Fe cofactors: R2lox and R2c proteins. *Journal of the American Chemical Society*, **2014**, 136, 13399-409	16.4	31
73	A main-group analogue of housene: the subtle influence of the inert-pair effect in group 15 clusters. *Angewandte Chemie - International Edition*, **2006**, 45, 6685-9	16.4	31
72	Structure and bonding in the isoelectronic series CnHnP5-n+: is phosphorus a carbon copy?. *Dalton Transactions*, **2004**, 2080-6	4.3	31

71	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 Hittorf's phosphorus. *Chemical Communications*, **2008**, 856-8	5.8	30
70	Cationic phosphorus-carbon-pnictogen cages isolobal to [C5R5]+. *Chemical Communications*, **2006**, 1375-7	3.8	30
69	Multireference Approaches to Spin-State Energetics of Transition Metal Complexes Utilizing the Density Matrix Renormalization Group. *Advanced Theory and Simulations*, **2019**, 2, 1800201	3.5	29
68	Redox potential tuning by redox-inactive cations in nature's water oxidizing catalyst and synthetic analogues. *Physical Chemistry Chemical Physics*, **2016**, 18, 10739-50	3.6	29
67	All-electron scalar relativistic basis sets for the elements Rb-Xe. *Journal of Computational Chemistry* , **2020**, 41, 1842-1849	3.5	28
66	A first-principles approach to the calculation of the on-site zero-field splitting in polynuclear transition metal complexes. *Inorganic Chemistry*, **2014**, 53, 11785-93	5.1	28
65	Accurate Computation of the Absorption Spectrum of Chlorophyll with Pair Natural Orbital Coupled Cluster Methods. *Journal of Physical Chemistry B*, **2020**, 124, 8761-8771	3.4	27
64	All-electron basis sets for heavy elements. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 363-374	7.9	26
63	Differences in the Active Site of Water Oxidation among Photosynthetic Organisms. *Journal of the American Chemical Society*, **2017**, 139, 14340-14343	16.4	25
62	Zwei ineinander umwandelbare Strukturen erklären die spektroskopischen Eigenschaften des Wasser oxidierenden Enzyms des Photosystems II im S2-Zustand. *Angewandte Chemie*, **2012**, 124, 10074-10079	3.6	25
61	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	6.4	25
60	C Coupling Constants, JCC, Are Reliable Probes for C Agostic Structures. *Organometallics*, **2009**, 28, 940-943	3.8	23
59	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, 12815-34	16.4	22
58	On the nature of the bonding in 1:1 adducts of O2. *Inorganic Chemistry*, **2003**, 42, 7734-6	5.1	22
57	Resolving the Manganese Oxidation States in the Oxygen-evolving Catalyst of Natural Photosynthesis. *Israel Journal of Chemistry*, **2015**, 55, 1219-1232	3.4	21
56	A re-evaluation of the two-step spin crossover in the trinuclear cation [Co3(dipyridylamido)4Cl2]+. *Dalton Transactions*, **2008**, 608-14	4.3	21
55	A new reaction pathway in organophosphorus chemistry: competing S(N)2 and AE' pathways for nucleophilic attack at a phosphorus-carbon cage compound. *Angewandte Chemie - International Edition*, **2006**, 45, 3628-31	16.4	21
54	Protein Matrix Control of Reaction Center Excitation in Photosystem II. *Journal of the American Chemical Society*, **2020**, 142, 18174-18190	16.4	21

53	Proton Translocation via Tautomerization of Asn298 During the S-S State Transition in the Oxygen-Evolving Complex of Photosystem II. *Journal of Physical Chemistry B*, **2019**, 123, 3068-3078	3.4	20
52	Concerted [2+2] cycloaddition of alkenes to a ruthenium-phosphorus double bond. *Angewandte Chemie - International Edition*, **2010**, 49, 3367-70	16.4	20
51	The S3 State of the Oxygen-Evolving Complex: Overview of Spectroscopy and XFEL Crystallography with a Critical Evaluation of Early-Onset Models for O□ Bond Formation. *Inorganics*, **2019**, 7, 55	2.9	19
50	Characterization of Oxygen Bridged Manganese Model Complexes Using Multifrequency (17)O-Hyperfine EPR Spectroscopies and Density Functional Theory. *Journal of Physical Chemistry B*, **2015**, 119, 13904-21	3.4	19
49	Benzonitrile Adducts of Terminal Diarylphosphido Complexes: Preparative Sources of □Ru?PR2□ *Organometallics*, **2011**, 30, 6458-6465	3.8	19
48	Synthesis and Computational Studies of Palladium(I) Dimers Pd2X2(PtBu2Ph)2(X = Br, I):□Phenyl versus Halide Bridging Modes. *Organometallics*, **2006**, 25, 5990-5995	3.8	18
47	Isolation and reactivity of an elusive diazoalkene. *Nature Chemistry*, **2021**, 13, 587-593	17.6	18
46	Axial ligand effect on the catalytic activity of biomimetic Fe-porphyrin catalyst: An experimental and DFT study. *Journal of Catalysis*, **2016**, 344, 768-777	7.3	18
45	Accurate Spin-State Energetics for Aryl Carbenes. *Journal of Chemical Theory and Computation*, **2018**, 14, 4733-4746	6.4	17
44	A Main-Group Analogue of Housene: The Subtle Influence of the Inert-Pair Effect in Group 15 Clusters. *Angewandte Chemie*, **2006**, 118, 6837-6841	3.6	16
43	Calcium and heterometallic manganese-calcium complexes supported by tripodal pyridine-carboxylate ligands: structural, EPR and theoretical investigations. *Dalton Transactions*, **2015**, 44, 12757-70	4.3	14
42	A New Reaction Pathway in Organophosphorus Chemistry: Competing SN2 and AE? Pathways for Nucleophilic Attack at a Phosphorus□arbon Cage Compound. *Angewandte Chemie*, **2006**, 118, 3710-3713	3.6	14
41	Arrested Substrate Binding Resolves Catalytic Intermediates in Higher-Plant Water Oxidation. *Angewandte Chemie - International Edition*, **2021**, 60, 3156-3162	16.4	14
40	Implications of structural heterogeneity for the electronic structure of the final oxygen-evolving intermediate in photosystem II. *Journal of Inorganic Biochemistry*, **2019**, 199, 110797	4.2	13
39	Orientational Jahn-Teller Isomerism in the Dark-Stable State of Nature's Water Oxidase. *Angewandte Chemie - International Edition*, **2021**, 60, 13493-13499	16.4	13
38	Orbital Entanglement Analysis of Exchange-Coupled Systems. *Journal of Physical Chemistry Letters*, **2019**, 10, 6762-6770	6.4	12
37	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	16.4	12
36	Understanding and tuning the properties of redox-accumulating manganese helicates. *Dalton Transactions*, **2016**, 45, 18900-18908	4.3	12

35	Assessment of Double-Hybrid Density Functional Theory for Magnetic Exchange Coupling in Manganese Complexes. *Inorganics*, **2019**, 7, 57	2.9	11
34	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	2.8	11
33	Accurate computed spin-state energetics for Co(iii) complexes: implications for modelling homogeneous catalysis. *Dalton Transactions*, **2020**, 49, 6478-6487	4.3	11
32	Theoretical Study on the Mechanism of Reaction of Ground-State Fe Atoms with Carbon Dioxide. *Collection of Czechoslovak Chemical Communications*, **2004**, 69, 13-33		11
31	Performance of density functional theory and orbital-optimised second-order perturbation theory methods for geometries and singlet–triplet state splittings of aryl-carbenes. *Molecular Physics*, **2020**, 118, e1764644	1.7	10
30	Promotion of phosphaalkyne cyclooligomerisation by a Sb(v) to Sb(iii) redox process. *Dalton Transactions*, **2008**, 3753-8	4.3	10
29	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	2.8	9
28	Alkene Insertions into a Ru–PR2 Bond. *Organometallics*, **2016**, 35, 3970-3980	3.8	9
27	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	5.1	9
26	Comparison of Density Functional and Correlated Wave Function Methods for the Prediction of Cu(II) Hyperfine Coupling Constants. *ChemPhysChem*, **2020**, 21, 2667-2679	3.2	8
25	Redox Isomerism in the S State of the Oxygen-Evolving Complex Resolved by Coupled Cluster Theory. *Chemistry - A European Journal*, **2021**, 27, 12815-12825	4.8	8
24	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 S2State. *Journal of the American Chemical Society*, **2011**, 133, 14149-14149	16.4	7
23	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	6.4	7
22	Evaluation of new low-valent computational models for the oxygen-evolving complex of photosystem II. *Chemical Physics Letters*, **2020**, 753, 137629	2.5	6
21	Structure-Spectroscopy Correlations for Intermediate Q of Soluble Methane Monooxygenase: Insights from QM/MM Calculations. *Journal of the American Chemical Society*, **2021**, 143, 6560-6577	16.4	6
20	Successes, challenges, and opportunities for quantum chemistry in understanding metalloenzymes for solar fuels research. *Chemical Communications*, **2021**, 57, 3952-3974	5.8	6
19	Systematic High-Accuracy Prediction of Electron Affinities for Biological Quinones. *Journal of Computational Chemistry*, **2018**, 39, 2439-2451	3.5	6
18	Applications of the Density Matrix Renormalization Group to Exchange-Coupled Transition Metal Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 91-120	0.7	5

17	Unusual P Hyperfine Strain Effects in a Conformationally Flexible Cu(II) Complex Revealed by Two-Dimensional Pulse EPR Spectroscopy. *Inorganic Chemistry*, **2020**, 59, 3666-3676	5.1	5
16	Oxygen-evolving Photosystem II **2014**, 1-13		4
15	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	3.1	4
14	Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. *Inorganic Chemistry*, **2021**, 60, 7399-7412	5.1	3
13	Arrested Substrate Binding Resolves Catalytic Intermediates in Higher-Plant Water Oxidation. *Angewandte Chemie*, **2021**, 133, 3193-3199	3.6	3
12	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	9.4	3
11	Spin-state energetics of manganese spin crossover complexes: Comparison of single-reference and multi-reference ab initio approaches. *Polyhedron*, **2021**, 208, 115399	2.7	3
10	Natural and Artificial Photosynthesis **2021**, 41-76		2
9	Orientational Jahn□Teller Isomerism in the Dark-Stable State of Nature's Water Oxidase. *Angewandte Chemie*, **2021**, 133, 13605-13611	3.6	2
8	The Reactivity of the Imine Bond within Polynuclear Nickel(II) Complexes. *Crystals*, **2021**, 11, 512	2.3	1
7	Reversible Silylium Transfer between P-H and Si-H Donors. *Angewandte Chemie - International Edition*, **2021**, 60, 2379-2384	16.4	1
6	Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled cluster theory. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9	1
5	Reversible Silylium Transfer between P-H and Si-H Donors. *Angewandte Chemie*, **2021**, 133, 2409-2414	3.6	0
4	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. *Magnetochemistry*, **2022**, 8, 36	3.1	0
3	Characterization of a Triplet Vinylidene.. *Journal of the American Chemical Society*, **2021**, 143, 21410-21416	15.4	0
2	Electrostatic profiling of photosynthetic pigments: implications for directed spectral tuning. *Physical Chemistry Chemical Physics*, **2021**, 23, 24677-24684	3.6	
1	Electronic properties of the S□=□5/2 Mn(II) complexes [Mn{PhC(O)NP(O)PPh2}(N,N)(NO3)], (N,N)□=□phenanthroline, neocuproine, 2,2?-bipyridine. *Polyhedron*, **2021**, 207, 115374	2.7	