

Victor S Batista

List of Publications by Year in descending order

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276
papers

14,391
citations

18887

64
h-index

32181

105
g-index

287
all docs

287
docs citations

287
times ranked

17721
citing authors

#	ARTICLE	IF	CITATIONS
1	Distinct allosteric pathways in imidazole glycerol phosphate synthase from yeast and bacteria. <i>Biophysical Journal</i> , 2022, 121, 119-130.	0.2	8
2	Binding of the substrate analog methanol in the oxygen-evolving complex of photosystem II in the D1-N87A genetic variant of cyanobacteria. <i>Faraday Discussions</i> , 2022, 234, 195-213.	1.6	4
3	Protein nanowires with tunable functionality and programmable self-assembly using sequence-controlled synthesis. <i>Nature Communications</i> , 2022, 13, 829.	5.8	30
4	High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, <i>Synechocystis</i> sp. PCC 6803. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	58
5	Insights into Binding of Single-Stranded Viral RNA Template to the Replication-Transcription Complex of SARS-CoV-2 for the Priming Reaction from Molecular Dynamics Simulations. <i>Biochemistry</i> , 2022, 61, 424-432.	1.2	10
6	MptpA Kinetics Enhanced by Allosteric Control of an Active Conformation. <i>Journal of Molecular Biology</i> , 2022, 434, 167540.	2.0	7
7	Functional Tensor-Train Chebyshev Method for Multidimensional Quantum Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 25-36.	2.3	10
8	Glycerol binding at the narrow channel of photosystem II stabilizes the low-spin S2 state of the oxygen-evolving complex. <i>Photosynthesis Research</i> , 2022, , 1.	1.6	1
9	Structural Basis for Reduced Dynamics of Three Engineered HNH Endonuclease Lys-to-Ala Mutants for the Clustered Regularly Interspaced Short Palindromic Repeat (CRISPR)-Associated 9 (CRISPR/Cas9) Enzyme. <i>Biochemistry</i> , 2022, 61, 785-794.	1.2	12
10	A 300-fold conductivity increase in microbial cytochrome nanowires due to temperature-induced restructuring of hydrogen bonding networks. <i>Science Advances</i> , 2022, 8, eabm7193.	4.7	28
11	Tensor-Train Split-Operator KSL (TT-SOKSL) Method for Quantum Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3327-3346.	2.3	9
12	Selective Heterogeneous Transfer Hydrogenation from Tertiary Amines to Alkynes. <i>ACS Catalysis</i> , 2021, 11, 5405-5415.	5.5	4
13	Tuning the Conduction Band for Interfacial Electron Transfer: Dye-Sensitized SnTiO ₂ Photoanodes for Water Splitting. <i>ACS Applied Energy Materials</i> , 2021, 4, 4695-4703.	2.5	4
14	Is Deprotonation of the Oxygen-Evolving Complex of Photosystem II during the S ₁ → S ₂ Transition Suppressed by Proton Quantum Delocalization?. <i>Journal of the American Chemical Society</i> , 2021, 143, 8324-8332.	6.6	21
15	Iterative Power Algorithm for Global Optimization with Quantics Tensor Trains. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3280-3291.	2.3	8
16	Introducing special issue on photocatalysis and photoelectrochemistry. <i>Journal of Chemical Physics</i> , 2021, 154, 190401.	1.2	0
17	Mechanism of Inhibition of the Reproduction of SARS-CoV-2 and Ebola Viruses by Remdesivir. <i>Biochemistry</i> , 2021, 60, 1869-1875.	1.2	12
18	Do crystallographic XFEL data support binding of a water molecule to the oxygen-evolving complex of photosystem II exposed to two flashes of light?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	11

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19	Proton exit pathways surrounding the oxygen evolving complex of photosystem II. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2021, 1862, 148446.	0.5	30
20	Observation of a potential-dependent switch of water-oxidation mechanism on Co-oxide-based catalysts. <i>CheM</i> , 2021, 7, 2101-2117.	5.8	42
21	Distorted Copper(II) Complex with Unusually Short CF ₂ -Cu Distances. <i>Inorganic Chemistry</i> , 2021, 60, 14759-14764.	1.9	1
22	A structurally preserved allosteric site in the MIF superfamily affects enzymatic activity and CD74 activation in D-dopachrome tautomerase. <i>Journal of Biological Chemistry</i> , 2021, 297, 101061.	1.6	7
23	Computational insights into the membrane fusion mechanism of SARS-CoV-2 at the cellular level. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 5019-5028.	1.9	10
24	Vibrational Stark shift spectroscopy of catalysts under the influence of electric fields at electrode-solution interfaces. <i>Chemical Science</i> , 2021, 12, 10131-10149.	3.7	25
25	Community Network Analysis of Allosteric Proteins. <i>Methods in Molecular Biology</i> , 2021, 2253, 137-151.	0.4	15
26	Intrinsic electronic conductivity of individual atomically resolved amyloid crystals reveals micrometer-long hole hopping via tyrosines. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	45
27	Nanotechnology for catalysis and solar energy conversion. <i>Nanotechnology</i> , 2021, 32, 042003.	1.3	44
28	Heterogeneous Composition of Oxygen-Evolving Complexes in Crystal Structures of Dark-Adapted Photosystem II. <i>Biochemistry</i> , 2021, 60, 3374-3384.	1.2	8
29	Development of an Enantioselective Synthesis of (S)-Euonyminol. <i>Journal of Organic Chemistry</i> , 2021, 86, 17011-17035.	1.7	6
30	Enhanced specificity mutations perturb allosteric signaling in CRISPR-Cas9. <i>ELife</i> , 2021, 10, .	2.8	27
31	Copper-mediated thiol potentiation and mutagenesis-guided modeling suggest a highly conserved copper-binding motif in human OR2M3. <i>Cellular and Molecular Life Sciences</i> , 2020, 77, 2157-2179.	2.4	29
32	Allosteric Motions of the CRISPR-Cas9 HNH Nuclease Probed by NMR and Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2020, 142, 1348-1358.	6.6	78
33	NMR and computational methods for molecular resolution of allosteric pathways in enzyme complexes. <i>Biophysical Reviews</i> , 2020, 12, 155-174.	1.5	35
34	Multihole water oxidation catalysis on haematite photoanodes revealed by operando spectroelectrochemistry and DFT. <i>Nature Chemistry</i> , 2020, 12, 82-89.	6.6	189
35	Ring-polymer, centroid, and mean-field approximations to multi-time Matsubara dynamics. <i>Journal of Chemical Physics</i> , 2020, 153, 124112.	1.2	11
36	Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast X-Ray Absorption Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20044-20048.	7.2	5

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37	Regulation of MIF Enzymatic Activity by an Allosteric Site at the Central Solvent Channel. <i>Cell Chemical Biology</i> , 2020, 27, 740-750.e5.	2.5	20
38	Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast X-ray Absorption Spectroscopy. <i>Angewandte Chemie</i> , 2020, 132, 20219-20223.	1.6	3
39	Two-dimensional Raman spectroscopy of Lennard-Jones liquids via ring-polymer molecular dynamics. <i>Journal of Chemical Physics</i> , 2020, 153, 034117.	1.2	9
40	D1-S169A substitution of photosystem II reveals a novel S2-state structure. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2020, 1861, 148301.	0.5	4
41	A conductive metal-organic framework photoanode. <i>Chemical Science</i> , 2020, 11, 9593-9603.	3.7	16
42	<i>In Situ</i> Identification of Reaction Intermediates and Mechanistic Understandings of Methane Oxidation over Hematite: A Combined Experimental and Theoretical Study. <i>Journal of the American Chemical Society</i> , 2020, 142, 17119-17130.	6.6	59
43	Electric field stimulates production of highly conductive microbial OmcZ nanowires. <i>Nature Chemical Biology</i> , 2020, 16, 1136-1142.	3.9	112
44	Efficient Multiphoton Sampling of Molecular Vibronic Spectra on a Superconducting Bosonic Processor. <i>Physical Review X</i> , 2020, 10, .	2.8	73
45	The Effect of (âˆ“)Epigallocatechin-3-Gallate on the Amyloid-Î² Secondary Structure. <i>Biophysical Journal</i> , 2020, 119, 349-359.	0.2	18
46	Semiconductor-to-conductor transition in 2D copper(II) oxide nanosheets through surface sulfur-functionalization. <i>Nanoscale</i> , 2020, 12, 14549-14559.	2.8	6
47	Surprisingly big linker-dependence of activity and selectivity in CO ₂ reduction by an iridium(I) pincer complex. <i>Chemical Communications</i> , 2020, 56, 9126-9129.	2.2	10
48	Identification of a Na ⁺ -Binding Site near the Oxygen-Evolving Complex of Spinach Photosystem II. <i>Biochemistry</i> , 2020, 59, 2823-2831.	1.2	5
49	Robust Binding of Disulfide-Substituted Rhenium Bipyridyl Complexes for CO ₂ Reduction on Gold Electrodes. <i>Frontiers in Chemistry</i> , 2020, 8, 86.	1.8	7
50	Decelerating Charge Recombination Using Fluorinated Porphyrins in <i>N,N</i> -Bis(3,4,5-trimethoxyphenyl)aniline-Aluminum(III) Porphyrin Fullerene Reaction Center Models. <i>Journal of the American Chemical Society</i> , 2020, 142, 10008-10024.	6.6	33
51	Allosteric Impact of the Variable Insert Loop in <i>Vaccinia</i> H1-Related (VHR) Phosphatase. <i>Biochemistry</i> , 2020, 59, 1896-1908.	1.2	5
52	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. <i>Journal of the American Chemical Society</i> , 2020, 142, 8403-8411.	6.6	35
53	Allosteric Control of Enzyme Activity: From Ancient Origins to Recent Gene-Editing Technologies. <i>Biochemistry</i> , 2020, 59, 1711-1712.	1.2	3
54	Facet-Dependent Kinetics and Energetics of Hematite for Solar Water Oxidation Reactions. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 5616-5622.	4.0	46

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55	Catalytic manganese oxide nanostructures for the reverse water gas shift reaction. <i>Nanoscale</i> , 2019, 11, 16677-16688.	2.8	31
56	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5837-5848.	1.1	2
57	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5973-5984.	1.2	1
58	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry C</i> , 2019, 123, 17063-17074.	1.5	1
59	The <i>JPC</i> Periodic Table. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4051-4062.	2.1	2
60	Multi-time formulation of Matsubara dynamics. <i>Journal of Chemical Physics</i> , 2019, 151, 034108.	1.2	14
61	Thermodynamics of the S ₂ -to-S ₃ state transition of the oxygen-evolving complex of photosystem II. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20840-20848.	1.3	21
62	Strongly Coupled Phenazine–Porphyrin Dyads: Light-Harvesting Molecular Assemblies with Broad Absorption Coverage. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 8000-8008.	4.0	36
63	D1-S169A Substitution of Photosystem II Perturbs Water Oxidation. <i>Biochemistry</i> , 2019, 58, 1379-1387.	1.2	18
64	Hammett neural networks: prediction of frontier orbital energies of tungsten–benzylidyne photoredox complexes. <i>Chemical Science</i> , 2019, 10, 6844-6854.	3.7	13
65	Chiral Inversion of Amino Acids in Antiparallel β -Sheets at Interfaces Probed by Vibrational Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5769-5781.	1.2	20
66	Vibronic Effects in the Ultrafast Interfacial Electron Transfer of Perylene-Sensitized TiO ₂ Surfaces. <i>Journal of Physical Chemistry C</i> , 2019, 123, 12599-12607.	1.5	15
67	Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations. <i>Accounts of Chemical Research</i> , 2019, 52, 1289-1300.	7.6	53
68	Search for Catalysts by Inverse Design: Artificial Intelligence, Mountain Climbers, and Alchemists. <i>Chemical Reviews</i> , 2019, 119, 6595-6612.	23.0	142
69	Regioselective Ultrafast Photoinduced Electron Transfer from Naphthols to Halocarbon Solvents. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2657-2662.	2.1	10
70	Effect of Electronic Coupling on Electron Transfer Rates from Photoexcited Naphthalenediimide Radical Anion to Re(bpy)(CO) ₃ X. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10178-10190.	1.5	10
71	Water Network Dynamics Next to the Oxygen-Evolving Complex of Photosystem II. <i>Inorganics</i> , 2019, 7, 39.	1.2	15
72	Collaboration between experiment and theory in solar fuels research. <i>Chemical Society Reviews</i> , 2019, 48, 1865-1873.	18.7	17

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73	Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3452-3461.	1.2	29
74	Relative stability of the S2 isomers of the oxygen evolving complex of photosystem II. <i>Photosynthesis Research</i> , 2019, 141, 331-341.	1.6	18
75	Atmospheric ¹² Caryophyllene-Derived Ozonolysis Products at Interfaces. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 158-169.	1.2	10
76	High-Energy Charge-Separated States by Reductive Electron Transfer Followed by Electron Shift in the Tetraphenylethylene- ¹⁸ Aluminum(III) Porphyrin- ¹⁹ Fullerene Triad. <i>Journal of Physical Chemistry C</i> , 2019, 123, 131-143.	1.5	24
77	Photoexcited radical anion super-reductants for solar fuels catalysis. <i>Coordination Chemistry Reviews</i> , 2018, 361, 98-119.	9.5	49
78	Floquet Study of Quantum Control of the Cis- ²⁰ Trans Photoisomerization of Rhodopsin. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1198-1205.	2.3	10
79	Nitrogen-doped tungsten carbide nanoarray as an efficient bifunctional electrocatalyst for water splitting in acid. <i>Nature Communications</i> , 2018, 9, 924.	5.8	571
80	Stable iridium dinuclear heterogeneous catalysts supported on metal-oxide substrate for solar water oxidation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2902-2907.	3.3	229
81	Nanosecond Dynamics Regulate the MIF-Induced Activity of CD74. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 7116-7119.	7.2	32
82	Molecular mechanism of activation of human musk receptors OR5AN1 and OR1A1 by (<i>R</i>) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3 Sciences of the United States of America, 2018, 115, E3950-E3958.	3.3	57
83	Direct Interfacial Electron Transfer from High-Potential Porphyrins into Semiconductor Surfaces: A Comparison of Linkers and Anchoring Groups. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13529-13539.	1.5	31
84	Investigating the Role of Copper Oxide in Electrochemical CO ₂ Reduction in Real Time. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 8574-8584.	4.0	207
85	Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. <i>Nature Communications</i> , 2018, 9, 415.	5.8	527
86	Hydrophobic CuO Nanosheets Functionalized with Organic Adsorbates. <i>Journal of the American Chemical Society</i> , 2018, 140, 1824-1833.	6.6	59
87	Can TDDFT Describe Excited Electronic States of Naphthol Photoacids? A Closer Look with EOM-CCSD. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 867-876.	2.3	27
88	Classical Optimal Control for Energy Minimization Based On Diffeomorphic Modulation under Observable-Response-Preserving Homotopy. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3351-3362.	2.3	4
89	Phenothiazine Radical Cation Excited States as Super-oxidants for Energy-Demanding Reactions. <i>Journal of the American Chemical Society</i> , 2018, 140, 5290-5299.	6.6	89
90	Carbon chain shape selectivity by the mouse olfactory receptor OR-17. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 2541-2548.	1.5	10

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91	Dopant-Dependent SFG Response of Rhenium CO ₂ Reduction Catalysts Chemisorbed on SrTiO ₃ (100) Single Crystals. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13944-13952.	1.5	10
92	Mechanistic study of CO/CO ₂ conversion catalyzed by a biomimetic Ni(II)-iminothiolate complex. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25555.	1.0	2
93	Electron-Hole-Pair-Induced Vibrational Energy Relaxation of Rhenium Catalysts on Gold Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 406-412.	2.1	22
94	Inverse Design of a Catalyst for Aqueous CO/CO ₂ Conversion Informed by the Ni ^{II} -iminothiolate Complex. <i>Inorganic Chemistry</i> , 2018, 57, 15474-15480.	1.9	13
95	CO ₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields. <i>Journal of the American Chemical Society</i> , 2018, 140, 17643-17655.	6.6	103
96	Eigenvector centrality for characterization of protein allosteric pathways. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E12201-E12208.	3.3	145
97	Reduced Occupancy of the Oxygen-Evolving Complex of Photosystem II Detected in Cryo-Electron Microscopy Maps. <i>Biochemistry</i> , 2018, 57, 5925-5929.	1.2	3
98	The structural basis for cancer drug interactions with the catalytic and allosteric sites of SAMHD1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E10022-E10031.	3.3	30
99	Distinct Binding of Rhenium Catalysts on Nanostructured and Single-Crystalline TiO ₂ Surfaces Revealed by Two-Dimensional Sum Frequency Generation Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2018, 122, 26018-26031.	1.5	8
100	Unusual Stability of a Bacteriochlorin Electrocatalyst under Reductive Conditions. A Case Study on CO ₂ Conversion to CO. <i>ACS Catalysis</i> , 2018, 8, 10131-10136.	5.5	28
101	Key role of the REC lobe during CRISPR-Cas9 activation by $\hat{\sim}$ sensing $\hat{\sim}$ TM , $\hat{\sim}$ regulating $\hat{\sim}$ TM , and $\hat{\sim}$ locking $\hat{\sim}$ TM the catalytic HNH domain. <i>Quarterly Reviews of Biophysics</i> , 2018, 51, .	2.4	79
102	A Multispecific Investigation of the Metal Effect in Mammalian Odorant Receptors for Sulfur-Containing Compounds. <i>Chemical Senses</i> , 2018, 43, 357-366.	1.1	7
103	Ultrafast proton-assisted tunneling through ZrO ₂ in dye-sensitized SnO ₂ -core/ZrO ₂ -shell films. <i>Chemical Communications</i> , 2018, 54, 7971-7974.	2.2	5
104	End-On Bound Iridium Dinuclear Heterogeneous Catalysts on WO ₃ for Solar Water Oxidation. <i>ACS Central Science</i> , 2018, 4, 1166-1172.	5.3	69
105	Inclusion of nuclear quantum effects for simulations of nonlinear spectroscopy. <i>Journal of Chemical Physics</i> , 2018, 148, 244105.	1.2	16
106	Water-Nucleophilic Attack Mechanism for the Cu ^{II} (pyalk) ₂ Water-Oxidation Catalyst. <i>ACS Catalysis</i> , 2018, 8, 7952-7960.	5.5	37
107	Nanosecond Dynamics Regulate the MIF-Induced Activity of CD74. <i>Angewandte Chemie</i> , 2018, 130, 7234-7237.	1.6	2
108	Behavior of Ru ^{II} Water Oxidation Catalysts in Low Oxidation States. <i>Chemistry - A European Journal</i> , 2018, 24, 12838-12847.	1.7	27

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109	Orientations of nonlocal vibrational modes from combined experimental and theoretical sum frequency spectroscopy. <i>Chemical Physics Letters</i> , 2017, 683, 199-204.	1.2	8
110	Energetics of the S ₂ State Spin Isomers of the Oxygen-Evolving Complex of Photosystem II. <i>Journal of Physical Chemistry B</i> , 2017, 121, 1020-1025.	1.2	38
111	Insights into Photosystem II from Isomorphous Difference Fourier Maps of Femtosecond X-ray Diffraction Data and Quantum Mechanics/Molecular Mechanics Structural Models. <i>ACS Energy Letters</i> , 2017, 2, 397-407.	8.8	16
112	Electrochemical Reduction of CO ₂ Catalyzed by Re(pyridine-oxazoline)(CO) ₃ Cl Complexes. <i>Inorganic Chemistry</i> , 2017, 56, 3214-3226.	1.9	48
113	Photoinduced electron transfer from rylene diimide radical anions and dianions to Re(bpy)(CO) ₃ using red and near-infrared light. <i>Chemical Science</i> , 2017, 8, 3821-3831.	3.7	57
114	Altering the allosteric pathway in IGPS suppresses millisecond motions and catalytic activity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E3414-E3423.	3.3	55
115	Inferring Protonation States of Hydroxamate Adsorbates on TiO ₂ Surfaces. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11985-11990.	1.5	5
116	The role of metals in mammalian olfaction of low molecular weight organosulfur compounds. <i>Natural Product Reports</i> , 2017, 34, 529-557.	5.2	33
117	Ultrafast photo-induced charge transfer of 1-naphthol and 2-naphthol to halocarbon solvents. <i>Chemical Physics Letters</i> , 2017, 683, 49-56.	1.2	8
118	Mechanistic Insights into Surface Chemical Interactions between Lithium Polysulfides and Transition Metal Oxides. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14222-14227.	1.5	86
119	Antimony Complexes for Electrocatalysis: Activity of a Main-Group Element in Proton Reduction. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9111-9115.	7.2	51
120	Interfacial Electron Transfer Followed by Photooxidation in <i>N,N</i> -Bis(<i>p</i> -anisole)aminopyridine-Aluminum(III) Porphyrin-Titanium(IV) Oxide Self-Assembled Photoanodes. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14484-14497.	1.5	12
121	Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants. <i>Journal of Chemical Physics</i> , 2017, 146, 215104.	1.2	6
122	Effects of aligned α -helix peptide dipoles on experimental electrostatic potentials. <i>Protein Science</i> , 2017, 26, 1692-1697.	3.1	7
123	Unanticipated Stickiness of α -Pinene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 3239-3246.	1.1	14
124	Ultrathin dendrimer-graphene oxide composite film for stable cycling lithium-sulfur batteries. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 3578-3583.	3.3	90
125	Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid. <i>Biochemistry</i> , 2017, 56, 96-106.	1.2	18
126	The O ₂ -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. <i>Accounts of Chemical Research</i> , 2017, 50, 41-48.	7.6	168

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127	Thousandfold Enhancement of Photoreduction Lifetime in $\text{Re}(\text{bpy})(\text{CO})_3$ via Spin-Dependent Electron Transfer from a Perylene diimide Radical Anion Donor. <i>Journal of the American Chemical Society</i> , 2017, 139, 16466-16469.	6.6	20
128	On the relationship between cumulative correlation coefficients and the quality of crystallographic data sets. <i>Protein Science</i> , 2017, 26, 2410-2416.	3.1	7
129	Robust resistive memory devices using solution-processable metal-coordinated azo aromatics . <i>Nature Materials</i> , 2017, 16, 1216-1224.	13.3	244
130	Electronic π -Delocalization Boosts Catalytic Water Oxidation by $\text{Cu}(\text{II})$ Molecular Catalysts Heterogenized on Graphene Sheets. <i>Journal of the American Chemical Society</i> , 2017, 139, 12907-12910.	6.6	108
131	X-ray Free Electron Laser Radiation Damage through the S-State Cycle of the Oxygen-Evolving Complex of Photosystem II. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9382-9388.	1.2	14
132	Crystallographic Data Support the Carousel Mechanism of Water Supply to the Oxygen-Evolving Complex of Photosystem II. <i>ACS Energy Letters</i> , 2017, 2, 2299-2306.	8.8	58
133	Linker Length-Dependent Electron-Injection Dynamics of Trimesitylporphyrins on SnO_2 Films. <i>Journal of Physical Chemistry C</i> , 2017, 121, 22690-22699.	1.5	13
134	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. <i>Journal of the American Chemical Society</i> , 2017, 139, 16028-16031.	6.6	104
135	Antimony Complexes for Electrocatalysis: Activity of a Main group Element in Proton Reduction. <i>Angewandte Chemie</i> , 2017, 129, 9239-9243.	1.6	12
136	Charge Transport and Rectification in Donor acceptor Dyads. <i>Journal of Physical Chemistry C</i> , 2017, 121, 19053-19062.	1.5	20
137	Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method: Multidimensional Nonadiabatic Quantum Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4034-4042.	2.3	84
138	Hard templating ultrathin polycrystalline hematite nanosheets: effect of nano-dimension on CO_2 to CO conversion via the reverse water-gas shift reaction. <i>Nanoscale</i> , 2017, 9, 12984-12995.	2.8	36
139	Interfacial Structure and Electric Field Probed by <i>in Situ</i> Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18674-18682.	1.5	77
140	Characterization of ammonia binding to the second coordination shell of the oxygen-evolving complex of photosystem II. <i>Dalton Transactions</i> , 2017, 46, 16089-16095.	1.6	12
141	Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6000-6009.	2.3	41
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