Victor S Batista

List of Publications by Year
in descending order

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276	14,391	16451 64	28297 105
papers	citations	h-index	g-index

287	287	287	15497
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Nitrogen-doped tungsten carbide nanoarray as an efficient bifunctional electrocatalyst for water splitting in acid. Nature Communications, 2018, 9, 924.	12.8	571
2	Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. Nature Communications, 2018, 9, 415.	12.8	527
3	Electrochemical CO₂ Reduction to Hydrocarbons on a Heterogeneous Molecular Cu Catalyst in Aqueous Solution. Journal of the American Chemical Society, 2016, 138, 8076-8079.	13.7	450
4	Quantum Dynamics Simulations of Interfacial Electron Transfer in Sensitized TiO2Semiconductors. Journal of the American Chemical Society, 2003, 125, 7989-7997.	13.7	368
5	Quantum Mechanics/Molecular Mechanics Study of the Catalytic Cycle of Water Splitting in Photosystem II. Journal of the American Chemical Society, 2008, 130, 3428-3442.	13.7	345
6	Light-driven water oxidation for solar fuels. Coordination Chemistry Reviews, 2012, 256, 2503-2520.	18.8	337
7	Intramolecular Proton Transfer Boosts Water Oxidation Catalyzed by a Ru Complex. Journal of the American Chemical Society, 2015, 137, 10786-10795.	13.7	246
8	Robust resistive memory devices using solution-processable metal-coordinated azoÂaromatics. Nature Materials, 2017, 16, 1216-1224.	27.5	244
9	Facet-Dependent Photoelectrochemical Performance of TiO₂ Nanostructures: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 1520-1529.	13.7	242
10	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.	7.1	229
11	S₁-State Model of the O₂-Evolving Complex of Photosystem II. Biochemistry, 2011, 50, 6308-6311.	2.5	210
12	Investigating the Role of Copper Oxide in Electrochemical CO₂ Reduction in Real Time. ACS Applied Materials & Interfaces, 2018, 10, 8574-8584.	8.0	207
13	Influence of Thermal Fluctuations on Interfacial Electron Transfer in Functionalized TiO2 Semiconductors. Journal of the American Chemical Society, 2005, 127, 18234-18242.	13.7	196
14	Allosteric pathways in imidazole glycerol phosphate synthase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E1428-36.	7.1	192
15	Multihole water oxidation catalysis on haematite photoanodes revealed by operando spectroelectrochemistry and DFT. Nature Chemistry, 2020, 12, 82-89.	13.6	189
16	The O₂-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.	15.6	168
17	Acetylacetonate Anchors for Robust Functionalization of TiO₂Nanoparticles with Mn(II)â^'Terpyridine Complexes. Journal of the American Chemical Society, 2008, 130, 14329-14338.	13.7	151
18	Functional Role of Pyridinium during Aqueous Electrochemical Reduction of CO₂ on Pt(111). Journal of Physical Chemistry Letters, 2013, 4, 745-748.	4.6	146

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19	Reduction of Systematic Uncertainty in DFT Redox Potentials of Transition-Metal Complexes. Journal of Physical Chemistry C, 2012, 116, 6349-6356.	3.1	145
20	Eigenvector centrality for characterization of protein allosteric pathways. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E12201-E12208.	7.1	145
21	Search for Catalysts by Inverse Design: Artificial Intelligence, Mountain Climbers, and Alchemists. Chemical Reviews, 2019, 119, 6595-6612.	47.7	142
22	Semiclassical molecular dynamics simulations of excited state double-proton transfer in 7-azaindole dimers. Journal of Chemical Physics, 1999, 110, 9922-9936.	3.0	138
23	QM/MM Models of the O2-Evolving Complex of Photosystem II. Journal of Chemical Theory and Computation, 2006, 2, 1119-1134.	5.3	136
24	Structuralâ€“Functional Role of Chloride in Photosystem II. Biochemistry, 2011, 50, 6312-6315.	2.5	132
25	Electric field stimulates production of highly conductive microbial OmcZ nanowires. Nature Chemical Biology, 2020, 16, 1136-1142.	8.0	112
26	A Model of the Oxygen-Evolving Center of Photosystem II Predicted by Structural Refinement Based on EXAFS Simulations. Journal of the American Chemical Society, 2008, 130, 6728-6730.	13.7	110
27	Electronic Ï€-Delocalization Boosts Catalytic Water Oxidation by Cu(II) Molecular Catalysts Heterogenized on Graphene Sheets. Journal of the American Chemical Society, 2017, 139, 12907-12910.	13.7	108
28	Covalent Attachment of a Rhenium Bipyridyl CO₂ Reduction Catalyst to Rutile TiO₂. Journal of the American Chemical Society, 2011, 133, 6922-6925.	13.7	106
29	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. Journal of the American Chemical Society, 2017, 139, 16028-16031.	13.7	104
30	CO₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields. Journal of the American Chemical Society, 2018, 140, 17643-17655.	13.7	103
31	Hydroxamate Anchors for Improved Photoconversion in Dye-Sensitized Solar Cells. Inorganic Chemistry, 2013, 52, 6752-6764.	4.0	102
32	Characterization of synthetic oxomanganese complexes and the inorganic core of the O2-evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. Journal of Inorganic Biochemistry, 2006, 100, 786-800.	3.5	99
33	Water-stable, hydroxamate anchors for functionalization of TiO2 surfaces with ultrafast interfacial electron transfer. Energy and Environmental Science, 2010, 3, 917.	30.8	99
34	QM/MM Study of Energy Storage and Molecular Rearrangements Due to the Primary Event in Vision. Biophysical Journal, 2004, 87, 2931-2941.	0.5	98
35	S₀-State Model of the Oxygen-Evolving Complex of Photosystem II. Biochemistry, 2013, 52, 7703-7706.	2.5	97
36	Hydroxamate anchors for water-stable attachment to TiO2 nanoparticles. Energy and Environmental Science, 2009, 2, 1173.	30.8	91

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37	Ultrathin dendrimerâ€“graphene oxide composite film for stable cycling lithiumâ€“sulfur batteries. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3578-3583.	7.1	90
38	Phenothiazine Radical Cation Excited States as Super-oxidants for Energy-Demanding Reactions. Journal of the American Chemical Society, 2018, 140, 5290-5299.	13.7	89
39	A tridentate Ni pincer for aqueous electrocatalytic hydrogen production. New Journal of Chemistry, 2012, 36, 1149.	2.8	88
40	Mechanistic Insights into Surface Chemical Interactions between Lithium Polysulfides and Transition Metal Oxides. Journal of Physical Chemistry C, 2017, 121, 14222-14227.	3.1	86
41	Role of Tensorial Electronic Friction in Energy Transfer at Metal Surfaces. Physical Review Letters, 2016, 116, 217601.	7.8	85
42	Femtosecond photoelectron spectroscopy of the I2â^' anion: A semiclassical molecular dynamics simulation method. Journal of Chemical Physics, 1999, 110, 3736-3747.	3.0	84
43	Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method: Multidimensional Nonadiabatic Quantum Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 4034-4042.	5.3	84
44	Ultrafast Photooxidation of Mn(II)â^'Terpyridine Complexes Covalently Attached to TiO₂ Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 11982-11990.	3.1	82
45	A Selfâ€Improved Waterâ€Oxidation Catalyst: Is One Site Really Enough?. Angewandte Chemie - International Edition, 2014, 53, 205-209.	13.8	82
46	Deposition of an oxomanganese water oxidation catalyst on TiO2 nanoparticles: computational modeling, assembly and characterization. Energy and Environmental Science, 2009, 2, 230.	30.8	80
47	Inverse Design and Synthesis of acac-Coumarin Anchors for Robust TiO₂ Sensitization. Journal of the American Chemical Society, 2011, 133, 9014-9022.	13.7	79
48	Heterogenized Iridium Water-Oxidation Catalyst from a Silatrane Precursor. ACS Catalysis, 2016, 6, 5371-5377.	11.2	79
49	Key role of the REC lobe during CRISPRâ€“Cas9 activation by â€˜sensingâ€™, â€˜regulatingâ€™, and â€˜lockingâ€™ the catalytic HNH domain. Quarterly Reviews of Biophysics, 2018, 51, .	5.7	79
50	Behavior of the Ru-bda Water Oxidation Catalyst Covalently Anchored on Glassy Carbon Electrodes. ACS Catalysis, 2015, 5, 3422-3429.	11.2	78
51	Allosteric Motions of the CRISPRâ€“Cas9 HNH Nuclease Probed by NMR and Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 1348-1358.	13.7	78
52	Matching-pursuit for simulations of quantum processes. Journal of Chemical Physics, 2003, 118, 6720-6724.	3.0	77
53	Interfacial Structure and Electric Field Probed by in Situ Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling. Journal of Physical Chemistry C, 2017, 121, 18674-18682.	3.1	77
54	Implausibility of the vibrational theory of olfaction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2766-74.	7.1	76

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55	Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. Accounts of Chemical Research, 2006, 39, 184-193.	15.6	75
56	Chiral Sum Frequency Generation for In Situ Probing Proton Exchange in Antiparallel Î²-Sheets at Interfaces. Journal of the American Chemical Society, 2013, 135, 3592-3598.	13.7	74
57	Ab initiotensorial electronic friction for molecules on metal surfaces: Nonadiabatic vibrational relaxation. Physical Review B, 2016, 94, .	3.2	74
58	Analysis of the Radiation-Damage-Free X-ray Structure of Photosystem II in Light of EXAFS and QM/MM Data. Biochemistry, 2015, 54, 1713-1716.	2.5	73
59	Efficient Multiphoton Sampling of Molecular Vibronic Spectra on a Superconducting Bosonic Processor. Physical Review X, 2020, 10, .	8.9	73
60	Amphiphilic Adsorption of Human Islet Amyloid Polypeptide Aggregates to Lipid/Aqueous Interfaces. Journal of Molecular Biology, 2012, 421, 537-547.	4.2	71
61	QM/MM computational studies of substrate water binding to the oxygen-evolving centre of photosystem II. Philosophical Transactions of the Royal Society B: Biological Sciences, 2008, 363, 1149-1156.	4.0	70
62	Bioinspired High-Potential Porphyrin Photoanodes. Journal of Physical Chemistry C, 2012, 116, 4892-4902.	3.1	69
63	End-On Bound Iridium Dinuclear Heterogeneous Catalysts on WO₃ for Solar Water Oxidation. ACS Central Science, 2018, 4, 1166-1172.	11.3	69
64	NH₃ Binding to the S₂ State of the O₂-Evolving Complex of Photosystem II: Analogue to H₂O Binding during the S₂ â†' S₃ Transition. Biochemistry, 2015, 54, 5783-5786.	2.5	68
65	Semiclassical molecular dynamics simulations of ultrafast photodissociation dynamics associated with the Chappuis band of ozone. Journal of Chemical Physics, 1998, 108, 498-510.	3.0	65
66	Nonadiabatic photodissociation dynamics ofICNin the Ãƒ continuum: A semiclassical initial value representation study. Journal of Chemical Physics, 2000, 112, 5566-5575.	3.0	65
67	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, 5511-5514.	13.7	63
68	Computational insights into the O2-evolving complex of photosystem II. Photosynthesis Research, 2008, 97, 91-114.	2.9	62
69	S₃ State of the O₂-Evolving Complex of Photosystem II: Insights from QM/MM, EXAFS, and Femtosecond X-ray Diffraction. Biochemistry, 2016, 55, 981-984.	2.5	62
70	Matching-pursuit/split-operator-Fourier-transform simulations of excited-state nonadiabatic quantum dynamics in pyrazine. Journal of Chemical Physics, 2006, 125, 124313.	3.0	61
71	Characterization of Proton Coupled Electron Transfer in a Biomimetic Oxomanganese Complex: Evaluation of the DFT B3LYP Level of Theory. Journal of Chemical Theory and Computation, 2010, 6, 755-760.	5.3	61
72	Smelling Sulfur: Copper and Silver Regulate the Response of Human Odorant Receptor OR2T11 to Low-Molecular-Weight Thiols. Journal of the American Chemical Society, 2016, 138, 13281-13288.	13.7	60

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73	Semiclassical molecular dynamics simulations of intramolecular proton transfer in photoexcited 2-(2â€²-hydroxyphenyl)â€“oxazole. Journal of Chemical Physics, 2000, 113, 9510-9522.	3.0	59
74	Hydrophobic CuO Nanosheets Functionalized with Organic Adsorbates. Journal of the American Chemical Society, 2018, 140, 1824-1833.	13.7	59
75	In Situ Identification of Reaction Intermediates and Mechanistic Understandings of Methane Oxidation over Hematite: A Combined Experimental and Theoretical Study. Journal of the American Chemical Society, 2020, 142, 17119-17130.	13.7	59
76	Crystallographic Data Support the Carousel Mechanism of Water Supply to the Oxygen-Evolving Complex of Photosystem II. ACS Energy Letters, 2017, 2, 2299-2306.	17.4	58
77	High-resolution cryo-electron microscopy structure of photosystem II from the mesophilic cyanobacterium, Synechocystis sp. PCC 6803. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	58
78	Photoinduced electron transfer from rylenediimide radical anions and dianions to Re(bpy)(CO)₃ using red and near-infrared light. Chemical Science, 2017, 8, 3821-3831.	7.4	57
79	Molecular mechanism of activation of human musk receptors OR5AN1 and OR1A1 by (R) Tj ETQq1 1 0.784314 rgBT /Overlock Sciences of the United States of America, 2018, 115, E3950-E3958.	7.1	57
80	Efficiency of Interfacial Electron Transfer from Zn-Porphyrin Dyes into TiO₂ Correlated to the Linker Single Molecule Conductance. Journal of Physical Chemistry C, 2013, 117, 24462-24470.	3.1	55
81	Altering the allosteric pathway in IGPS suppresses millisecond motions and catalytic activity. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E3414-E3423.	7.1	55
82	Activation of OR1A1 suppresses PPAR-Î³ expression by inducing HES-1 in cultured hepatocytes. International Journal of Biochemistry and Cell Biology, 2015, 64, 75-80.	2.8	54
83	Real time path integrals using the Hermanâ€“Kluk propagator. Journal of Chemical Physics, 2002, 116, 2748-2756.	3.0	53
84	Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations. Accounts of Chemical Research, 2019, 52, 1289-1300.	15.6	53
85	Ultrafast Photoinduced Interfacial Proton Coupled Electron Transfer from CdSe Quantum Dots to 4,4â€²-Bipyridine. Journal of the American Chemical Society, 2016, 138, 884-892.	13.7	52
86	Coherent Control in the Presence of Intrinsic Decoherence: Proton Transfer in Large Molecular Systems. Physical Review Letters, 2002, 89, 143201.	7.8	51
87	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, 7243-7250.	13.7	51
88	Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie - International Edition, 2017, 56, 9111-9115.	13.8	51
89	Quantum tunneling dynamics in multidimensional systems: A matching-pursuit description. Journal of Chemical Physics, 2004, 121, 1676-1680.	3.0	50
90	Crucial Role of Nuclear Dynamics for Electron Injection in a Dyeâ€“Semiconductor Complex. Journal of Physical Chemistry Letters, 2015, 6, 2393-2398.	4.6	49

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91	Accurate Line Shapes from Sub-1 cm^{â€“1} Resolution Sum Frequency Generation Vibrational Spectroscopy of Î±-Pinene at Room Temperature. Journal of Physical Chemistry A, 2015, 119, 1292-1302.	2.5	49
92	Photoexcited radical anion super-reductants for solar fuels catalysis. Coordination Chemistry Reviews, 2018, 361, 98-119.	18.8	49
93	Orientation of a Series of CO2 Reduction Catalysts on Single Crystal TiO2 Probed by Phase-Sensitive Vibrational Sum Frequency Generation Spectroscopy (PS-VSFG). Journal of Physical Chemistry C, 2012, 116, 24107-24114.	3.1	48
94	Electrochemical Reduction of CO₂ Catalyzed by Re(pyridine-oxazoline)(CO)₃Cl Complexes. Inorganic Chemistry, 2017, 56, 3214-3226.	4.0	48
95	A Self-Consistent Space-Domain Decomposition Method for QM/MM Computations of Protein Electrostatic Potentials. Journal of Chemical Theory and Computation, 2006, 2, 175-186.	5.3	47
96	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.	10.3	47
97	Structural Changes in the Oxygen-Evolving Complex of PhotosystemÂII Induced by the S₁ to S₂ Transition: A Combined XRD and QM/MM Study. Biochemistry, 2014, 53, 6860-6862.	2.5	46
98	Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie - International Edition, 2016, 55, 14818-14822.	13.8	46
99	Orientation of Cyano-Substituted Bipyridine Re(I) fac-Tricarbonyl Electrocatalysts Bound to Conducting Au Surfaces. Journal of Physical Chemistry C, 2016, 120, 1657-1665.	3.1	46
100	Facet-Dependent Kinetics and Energetics of Hematite for Solar Water Oxidation Reactions. ACS Applied Materials & Interfaces, 2019, 11, 5616-5622.	8.0	46
101	QM/MM Study of the NMR Spectroscopy of the Retinyl Chromophore in Visual Rhodopsin. Journal of Chemical Theory and Computation, 2005, 1, 674-685.	5.3	45
102	Intrinsic electronic conductivity of individual atomically resolved amyloid crystals reveals micrometer-long hole hopping via tyrosines. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	45
103	Surface-Induced Anisotropic Binding of a Rhenium CO₂-Reduction Catalyst on Rutile TiO₂(110) Surfaces. Journal of Physical Chemistry C, 2016, 120, 20970-20977.	3.1	44
104	Nanotechnology for catalysis and solar energy conversion. Nanotechnology, 2021, 32, 042003.	2.6	44
105	Model study of coherent quantum dynamics of hole states in functionalized semiconductor nanostructures. Journal of Chemical Physics, 2005, 122, 154709.	3.0	43
106	Electrode-Ligand Interactions Dramatically Enhance CO₂ Conversion to CO by the [Ni(cyclam)](PF₆)₂ Catalyst. ACS Catalysis, 2017, 7, 5282-5288.	11.2	43
107	Experimental and Theoretical Study of CO₂ Insertion into Ruthenium Hydride Complexes. Inorganic Chemistry, 2016, 55, 1623-1632.	4.0	42
108	Observation of a potential-dependent switch of water-oxidation mechanism on Co-oxide-based catalysts. CheM, 2021, 7, 2101-2117.	11.7	42

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109	Mechanism of Manganese-Catalyzed Oxygen Evolution from Experimental and Theoretical Analyses of ¹⁸O Kinetic Isotope Effects. ACS Catalysis, 2015, 5, 7104-7113.	11.2	41
110	Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. Journal of Chemical Theory and Computation, 2017, 13, 6000-6009.	5.3	41
111	Allosteric Pathways in the PPARÎ³-RXRÎ± nuclear receptor complex. Scientific Reports, 2016, 6, 19940.	3.3	39
112	Fundamental Role of Oxygen Stoichiometry in Controlling the Band Gap and Reactivity of Cupric Oxide Nanosheets. Journal of the American Chemical Society, 2016, 138, 10978-10985.	13.7	39
113	Dissecting Dynamic Allosteric Pathways Using Chemically Related Small-Molecule Activators. Structure, 2016, 24, 1155-1166.	3.3	38
114	Energetics of the S₂ State Spin Isomers of the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2017, 121, 1020-1025.	2.6	38
115	Visible Light Sensitization of TiO₂ Surfaces with Alq3 Complexes. Journal of Physical Chemistry C, 2010, 114, 1317-1325.	3.1	37
116	Water-Nucleophilic Attack Mechanism for the Cu^{II}(pyalk)₂ Water-Oxidation Catalyst. ACS Catalysis, 2018, 8, 7952-7960.	11.2	37
117	Electrostatic Effects on Proton Coupled Electron Transfer in Oxomanganese Complexes Inspired by the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2013, 117, 6217-6226.	2.6	36
118	Single Molecule Rectification Induced by the Asymmetry of a Single Frontier Orbital. Journal of Chemical Theory and Computation, 2014, 10, 3393-3400.	5.3	36
119	Hard templating ultrathin polycrystalline hematite nanosheets: effect of nano-dimension on CO₂ to CO conversion via the reverse water-gas shift reaction. Nanoscale, 2017, 9, 12984-12995.	5.6	36
120	Strongly Coupled Phenazineâ€“Porphyrin Dyads: Light-Harvesting Molecular Assemblies with Broad Absorption Coverage. ACS Applied Materials & Interfaces, 2019, 11, 8000-8008.	8.0	36
121	Coherent Control of Quantum Dynamics with Sequences of Unitary Phase-Kick Pulses. Annual Review of Physical Chemistry, 2009, 60, 293-320.	10.8	35
122	Fuel selection for a regenerative organic fuel cell/flow battery: thermodynamic considerations. Energy and Environmental Science, 2012, 5, 9534.	30.8	35
123	NMR and computational methods for molecular resolution of allosteric pathways in enzyme complexes. Biophysical Reviews, 2020, 12, 155-174.	3.2	35
124	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. Journal of the American Chemical Society, 2020, 142, 8403-8411.	13.7	35
125	Computational Design of Intrinsic Molecular Rectifiers Based on Asymmetric Functionalization of N-Phenylbenzamide. Journal of Chemical Theory and Computation, 2015, 11, 5888-5896.	5.3	34
126	Controlling the rectification properties of molecular junctions through moleculeâ€“electrode coupling. Nanoscale, 2016, 8, 16357-16362.	5.6	33

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127	Allosteric Communication Disrupted by a Small Molecule Binding to the Imidazole Glycerol Phosphate Synthase Proteinâ€“Protein Interface. Biochemistry, 2016, 55, 6484-6494.	2.5	33
128	The role of metals in mammalian olfaction of low molecular weight organosulfur compounds. Natural Product Reports, 2017, 34, 529-557.	10.3	33
129	Decelerating Charge Recombination Using Fluorinated Porphyrins in N,N-Bis(3,4,5-trimethoxyphenyl)anilineâ€”Aluminum(III) Porphyrinâ€”Fullerene Reaction Center Models. Journal of the American Chemical Society, 2020, 142, 10008-10024.	13.7	33
130	Model Study of Coherent-Control of the Femtosecond Primary Event of Vision. Journal of Physical Chemistry B, 2004, 108, 6745-6749.	2.6	32
131	QM/MM Model of the Mouse Olfactory Receptor MOR244-3 Validated by Site-Directed Mutagenesis Experiments. Biophysical Journal, 2014, 107, L5-L8.	0.5	32
132	A full set of iridium(<scp>iv</scp>) pyridine-alkoxide stereoisomers: highly geometry-dependent redox properties. Chemical Science, 2017, 8, 1642-1652.	7.4	32
133	Nanosecond Dynamics Regulate the MIFâ€Induced Activity of CD74. Angewandte Chemie - International Edition, 2018, 57, 7116-7119.	13.8	32
134	Computational Insights on Crystal Structures of the Oxygen-Evolving Complex of Photosystem II with Either Ca²⁺ or Ca²⁺ Substituted by Sr²⁺. Biochemistry, 2015, 54, 820-825.	2.5	31
135	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.	3.1	31
136	Catalytic manganese oxide nanostructures for the reverse water gas shift reaction. Nanoscale, 2019, 11, 16677-16688.	5.6	31
137	Characterization of Parallel Î²-Sheets at Interfaces by Chiral Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry Letters, 2015, 6, 1310-1315.	4.6	30
138	Molecular titaniumâ€“hydroxamate complexes as models for TiO₂ surface binding. Chemical Communications, 2016, 52, 2972-2975.	4.1	30
139	The structural basis for cancer drug interactions with the catalytic and allosteric sites of SAMHD1. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10022-E10031.	7.1	30
140	Proton exit pathways surrounding the oxygen evolving complex of photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148446.	1.0	30
141	Protein nanowires with tunable functionality and programmable self-assembly using sequence-controlled synthesis. Nature Communications, 2022, 13, 829.	12.8	30
142	Ultrafast Vibrational Frequency Shifts Induced by Electronic Excitations: Naphthols in Low Dielectric Media. Journal of Physical Chemistry A, 2012, 116, 2775-2790.	2.5	29
143	Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of Î±-Pinene on Silica. Journal of Physical Chemistry C, 2016, 120, 12578-12589.	3.1	29
144	Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks. Journal of Physical Chemistry B, 2019, 123, 3452-3461.	2.6	29

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145	Copper-mediated thiol potentiation and mutagenesis-guided modeling suggest a highly conserved copper-binding motif in human OR2M3. Cellular and Molecular Life Sciences, 2020, 77, 2157-2179.	5.4	29
146	High-Potential Porphyrins Supported on SnO₂ and TiO₂ Surfaces for Photoelectrochemical Applications. Journal of Physical Chemistry C, 2016, 120, 28971-28982.	3.1	28
147	Unusual Stability of a Bacteriochlorin Electrocatalyst under Reductive Conditions. A Case Study on CO₂ Conversion to CO. ACS Catalysis, 2018, 8, 10131-10136.	11.2	28
148	A 300-fold conductivity increase in microbial cytochrome nanowires due to temperature-induced restructuring of hydrogen bonding networks. Science Advances, 2022, 8, eabm7193.	10.3	28
149	Unusual kinetics of thermal decay of dim-light photoreceptors in vertebrate vision. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10438-10443.	7.1	27
150	Can TDDFT Describe Excited Electronic States of Naphthol Photoacids? A Closer Look with EOM-CCSD. Journal of Chemical Theory and Computation, 2018, 14, 867-876.	5.3	27
151	Behavior of Ruâ€“bda Waterâ€Oxidation Catalysts in Low Oxidation States. Chemistry - A European Journal, 2018, 24, 12838-12847.	3.3	27
152	Enhanced specificity mutations perturb allosteric signaling in CRISPR-Cas9. ELife, 2021, 10, .	6.0	27
153	Theoretical EXAFS studies of a model of the oxygenâ€evolving complex of photosystem II obtained with the quantum cluster approach. International Journal of Quantum Chemistry, 2013, 113, 474-478.	2.0	26
154	Correlating Photoacidity to Hydrogen-Bond Structure by Using the Local Oâ€“H Stretching Probe in Hydrogen-Bonded Complexes of Aromatic Alcohols. Journal of Physical Chemistry A, 2015, 119, 4800-4812.	2.5	26
155	Quantitative structure-property relationship model leading to virtual screening of fullerene derivatives: Exploring structural attributes critical for photoconversion efficiency of polymer solar cell acceptors. Nano Energy, 2016, 26, 677-691.	16.0	25
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