Victor S Batista

List of Publications by Year
in descending order

276 papers	14,391 citations	16437 64 h-index	28275 105 g-index
287 all docs	287 docs citations	287 times ranked	15497 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.	5.8	571
2	Active sites of copper-complex catalytic materials for electrochemical carbon dioxide reduction. Nature Communications, 2018, 9, 415.	5.8	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.	6.6	450
4	Quantum Dynamics Simulations of Interfacial Electron Transfer in Sensitized TiO2Semiconductors. Journal of the American Chemical Society, 2003, 125, 7989-7997.	6.6	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.	6.6	345
6	Light-driven water oxidation for solar fuels. Coordination Chemistry Reviews, 2012, 256, 2503-2520.	9.5	337
7	Intramolecular Proton Transfer Boosts Water Oxidation Catalyzed by a Ru Complex. Journal of the American Chemical Society, 2015, 137, 10786-10795.	6.6	246
8	Robust resistive memory devices using solution-processable metal-coordinated azoÂaromatics. Nature Materials, 2017, 16, 1216-1224.	13.3	244
9	Facet-Dependent Photoelectrochemical Performance of TiO₂ Nanostructures: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 1520-1529.	6.6	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.	3.3	229
11	S₁-State Model of the O₂-Evolving Complex of Photosystem II. Biochemistry, 2011, 50, 6308-6311.	1.2	210
12	Investigating the Role of Copper Oxide in Electrochemical CO₂ Reduction in Real Time. ACS Applied Materials & Interfaces, 2018, 10, 8574-8584.	4.0	207
13	Influence of Thermal Fluctuations on Interfacial Electron Transfer in Functionalized TiO2 Semiconductors. Journal of the American Chemical Society, 2005, 127, 18234-18242.	6.6	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.	3.3	192
15	Multihole water oxidation catalysis on haematite photoanodes revealed by operando spectroelectrochemistry and DFT. Nature Chemistry, 2020, 12, 82-89.	6.6	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.	7.6	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.	6.6	151
18	Functional Role of Pyridinium during Aqueous Electrochemical Reduction of CO₂ on Pt(111). Journal of Physical Chemistry Letters, 2013, 4, 745-748.	2.1	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.	1.5	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.	3.3	145
21	Search for Catalysts by Inverse Design: Artificial Intelligence, Mountain Climbers, and Alchemists. Chemical Reviews, 2019, 119, 6595-6612.	23.0	142
22	Semiclassical molecular dynamics simulations of excited state double-proton transfer in 7-azaindole dimers. Journal of Chemical Physics, 1999, 110, 9922-9936.	1.2	138
23	QM/MM Models of the O2-Evolving Complex of Photosystem II. Journal of Chemical Theory and Computation, 2006, 2, 1119-1134.	2.3	136
24	Structuralâ€“Functional Role of Chloride in Photosystem II. Biochemistry, 2011, 50, 6312-6315.	1.2	132
25	Electric field stimulates production of highly conductive microbial OmcZ nanowires. Nature Chemical Biology, 2020, 16, 1136-1142.	3.9	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.	6.6	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.	6.6	108
28	Covalent Attachment of a Rhenium Bipyridyl CO₂ Reduction Catalyst to Rutile TiO₂. Journal of the American Chemical Society, 2011, 133, 6922-6925.	6.6	106
29	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. Journal of the American Chemical Society, 2017, 139, 16028-16031.	6.6	104
30	CO₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields. Journal of the American Chemical Society, 2018, 140, 17643-17655.	6.6	103
31	Hydroxamate Anchors for Improved Photoconversion in Dye-Sensitized Solar Cells. Inorganic Chemistry, 2013, 52, 6752-6764.	1.9	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.	1.5	99
33	Water-stable, hydroxamate anchors for functionalization of TiO2 surfaces with ultrafast interfacial electron transfer. Energy and Environmental Science, 2010, 3, 917.	15.6	99
34	QM/MM Study of Energy Storage and Molecular Rearrangements Due to the Primary Event in Vision. Biophysical Journal, 2004, 87, 2931-2941.	0.2	98
35	S₀-State Model of the Oxygen-Evolving Complex of Photosystem II. Biochemistry, 2013, 52, 7703-7706.	1.2	97
36	Hydroxamate anchors for water-stable attachment to TiO2 nanoparticles. Energy and Environmental Science, 2009, 2, 1173.	15.6	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.	3.3	90
38	Phenothiazine Radical Cation Excited States as Super-oxidants for Energy-Demanding Reactions. Journal of the American Chemical Society, 2018, 140, 5290-5299.	6.6	89
39	A tridentate Ni pincer for aqueous electrocatalytic hydrogen production. New Journal of Chemistry, 2012, 36, 1149.	1.4	88
40	Mechanistic Insights into Surface Chemical Interactions between Lithium Polysulfides and Transition Metal Oxides. Journal of Physical Chemistry C, 2017, 121, 14222-14227.	1.5	86
41	Role of Tensorial Electronic Friction in Energy Transfer at Metal Surfaces. Physical Review Letters, 2016, 116, 217601.	2.9	85
42	Femtosecond photoelectron spectroscopy of the I2â¯ anion: A semiclassical molecular dynamics simulation method. Journal of Chemical Physics, 1999, 110, 3736-3747.	1.2	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.	2.3	84
44	Ultrafast Photooxidation of Mn(II)â¯Terpyridine Complexes Covalently Attached to TiO₂ Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 11982-11990.	1.5	82
45	A Selfâ€Improved Waterâ€Oxidation Catalyst: Is One Site Really Enough?. Angewandte Chemie - International Edition, 2014, 53, 205-209.	7.2	82
46	Deposition of an oxomanganese water oxidation catalyst on TiO2 nanoparticles: computational modeling, assembly and characterization. Energy and Environmental Science, 2009, 2, 230.	15.6	80
47	Inverse Design and Synthesis of acac-Coumarin Anchors for Robust TiO₂ Sensitization. Journal of the American Chemical Society, 2011, 133, 9014-9022.	6.6	79
48	Heterogenized Iridium Water-Oxidation Catalyst from a Silatrane Precursor. ACS Catalysis, 2016, 6, 5371-5377.	5.5	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, .	2.4	79
50	Behavior of the Ru-bda Water Oxidation Catalyst Covalently Anchored on Glassy Carbon Electrodes. ACS Catalysis, 2015, 5, 3422-3429.	5.5	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.	6.6	78
52	Matching-pursuit for simulations of quantum processes. Journal of Chemical Physics, 2003, 118, 6720-6724.	1.2	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.	1.5	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.	3.3	76

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55	Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. Accounts of Chemical Research, 2006, 39, 184-193.	7.6	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.	6.6	74
57	Ab initiotensorial electronic friction for molecules on metal surfaces: Nonadiabatic vibrational relaxation. Physical Review B, 2016, 94, .	1.1	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.	1.2	73
59	Efficient Multiphoton Sampling of Molecular Vibronic Spectra on a Superconducting Bosonic Processor. Physical Review X, 2020, 10, .	2.8	73
60	Amphiphilic Adsorption of Human Islet Amyloid Polypeptide Aggregates to Lipid/Aqueous Interfaces. Journal of Molecular Biology, 2012, 421, 537-547.	2.0	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.	1.8	70
62	Bioinspired High-Potential Porphyrin Photoanodes. Journal of Physical Chemistry C, 2012, 116, 4892-4902.	1.5	69
63	End-On Bound Iridium Dinuclear Heterogeneous Catalysts on WO₃ for Solar Water Oxidation. ACS Central Science, 2018, 4, 1166-1172.	5.3	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.	1.2	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.	1.2	65
66	Nonadiabatic photodissociation dynamics ofICNin the Ãƒ continuum: A semiclassical initial value representation study. Journal of Chemical Physics, 2000, 112, 5566-5575.	1.2	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.	6.6	63
68	Computational insights into the O2-evolving complex of photosystem II. Photosynthesis Research, 2008, 97, 91-114.	1.6	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.	1.2	62
70	Matching-pursuit/split-operator-Fourier-transform simulations of excited-state nonadiabatic quantum dynamics in pyrazine. Journal of Chemical Physics, 2006, 125, 124313.	1.2	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.	2.3	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.	6.6	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.	1.2	59
74	Hydrophobic CuO Nanosheets Functionalized with Organic Adsorbates. Journal of the American Chemical Society, 2018, 140, 1824-1833.	6.6	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.	6.6	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.	8.8	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, .	3.3	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.	3.7	57
79	Molecular mechanism of activation of human musk receptors OR5AN1 and OR1A1 by (R) Tj ETQq1 1 0.784314 rgBT /Overlock 1 Sciences of the United States of America, 2018, 115, E3950-E3958.	3.3	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.	1.5	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.	3.3	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.	1.2	54
83	Real time path integrals using the Hermanâ€“Kluk propagator. Journal of Chemical Physics, 2002, 116, 2748-2756.	1.2	53
84	Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations. Accounts of Chemical Research, 2019, 52, 1289-1300.	7.6	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.	6.6	52
86	Coherent Control in the Presence of Intrinsic Decoherence: Proton Transfer in Large Molecular Systems. Physical Review Letters, 2002, 89, 143201.	2.9	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.	6.6	51
88	Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie - International Edition, 2017, 56, 9111-9115.	7.2	51
89	Quantum tunneling dynamics in multidimensional systems: A matching-pursuit description. Journal of Chemical Physics, 2004, 121, 1676-1680.	1.2	50
90	Crucial Role of Nuclear Dynamics for Electron Injection in a Dyeâ€“Semiconductor Complex. Journal of Physical Chemistry Letters, 2015, 6, 2393-2398.	2.1	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.	1.1	49
92	Photoexcited radical anion super-reductants for solar fuels catalysis. Coordination Chemistry Reviews, 2018, 361, 98-119.	9.5	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.	1.5	48
94	Electrochemical Reduction of CO₂ Catalyzed by Re(pyridine-oxazoline)(CO)₃Cl Complexes. Inorganic Chemistry, 2017, 56, 3214-3226.	1.9	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.	2.3	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.	5.2	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.	1.2	46
98	Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie - International Edition, 2016, 55, 14818-14822.	7.2	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.	1.5	46
100	Facet-Dependent Kinetics and Energetics of Hematite for Solar Water Oxidation Reactions. ACS Applied Materials & Interfaces, 2019, 11, 5616-5622.	4.0	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.	2.3	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, .	3.3	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.	1.5	44
104	Nanotechnology for catalysis and solar energy conversion. Nanotechnology, 2021, 32, 042003.	1.3	44
105	Model study of coherent quantum dynamics of hole states in functionalized semiconductor nanostructures. Journal of Chemical Physics, 2005, 122, 154709.	1.2	43
106	Electrode-Ligand Interactions Dramatically Enhance CO₂ Conversion to CO by the [Ni(cyclam)](PF₆)₂ Catalyst. ACS Catalysis, 2017, 7, 5282-5288.	5.5	43
107	Experimental and Theoretical Study of CO₂ Insertion into Ruthenium Hydride Complexes. Inorganic Chemistry, 2016, 55, 1623-1632.	1.9	42
108	Observation of a potential-dependent switch of water-oxidation mechanism on Co-oxide-based catalysts. CheM, 2021, 7, 2101-2117.	5.8	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.	5.5	41
110	Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. Journal of Chemical Theory and Computation, 2017, 13, 6000-6009.	2.3	41
111	Allosteric Pathways in the PPARÎ³-RXRÎ± nuclear receptor complex. Scientific Reports, 2016, 6, 19940.	1.6	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.	6.6	39
113	Dissecting Dynamic Allosteric Pathways Using Chemically Related Small-Molecule Activators. Structure, 2016, 24, 1155-1166.	1.6	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.	1.2	38
115	Visible Light Sensitization of TiO₂ Surfaces with Alq3 Complexes. Journal of Physical Chemistry C, 2010, 114, 1317-1325.	1.5	37
116	Water-Nucleophilic Attack Mechanism for the Cu^{II}(pyalk)₂ Water-Oxidation Catalyst. ACS Catalysis, 2018, 8, 7952-7960.	5.5	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.	1.2	36
118	Single Molecule Rectification Induced by the Asymmetry of a Single Frontier Orbital. Journal of Chemical Theory and Computation, 2014, 10, 3393-3400.	2.3	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.	2.8	36
120	Strongly Coupled Phenazineâ€“Porphyrin Dyads: Light-Harvesting Molecular Assemblies with Broad Absorption Coverage. ACS Applied Materials & Interfaces, 2019, 11, 8000-8008.	4.0	36
121	Coherent Control of Quantum Dynamics with Sequences of Unitary Phase-Kick Pulses. Annual Review of Physical Chemistry, 2009, 60, 293-320.	4.8	35
122	Fuel selection for a regenerative organic fuel cell/flow battery: thermodynamic considerations. Energy and Environmental Science, 2012, 5, 9534.	15.6	35
123	NMR and computational methods for molecular resolution of allosteric pathways in enzyme complexes. Biophysical Reviews, 2020, 12, 155-174.	1.5	35
124	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. Journal of the American Chemical Society, 2020, 142, 8403-8411.	6.6	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.	2.3	34
126	Controlling the rectification properties of molecular junctions through moleculeâ€“electrode coupling. Nanoscale, 2016, 8, 16357-16362.	2.8	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.	1.2	33
128	The role of metals in mammalian olfaction of low molecular weight organosulfur compounds. Natural Product Reports, 2017, 34, 529-557.	5.2	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.	6.6	33
130	Model Study of Coherent-Control of the Femtosecond Primary Event of Vision. Journal of Physical Chemistry B, 2004, 108, 6745-6749.	1.2	32
131	QM/MM Model of the Mouse Olfactory Receptor MOR244-3 Validated by Site-Directed Mutagenesis Experiments. Biophysical Journal, 2014, 107, L5-L8.	0.2	32
132	A full set of iridium(<scp>iv</scp>) pyridine-alkoxide stereoisomers: highly geometry-dependent redox properties. Chemical Science, 2017, 8, 1642-1652.	3.7	32
133	Nanosecond Dynamics Regulate the MIFâ€Induced Activity of CD74. Angewandte Chemie - International Edition, 2018, 57, 7116-7119.	7.2	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.	1.2	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.	1.5	31
136	Catalytic manganese oxide nanostructures for the reverse water gas shift reaction. Nanoscale, 2019, 11, 16677-16688.	2.8	31
137	Characterization of Parallel Î²-Sheets at Interfaces by Chiral Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry Letters, 2015, 6, 1310-1315.	2.1	30
138	Molecular titaniumâ€“hydroxamate complexes as models for TiO₂ surface binding. Chemical Communications, 2016, 52, 2972-2975.	2.2	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.	3.3	30
140	Proton exit pathways surrounding the oxygen evolving complex of photosystem II. Biochimica Et Biophysica Acta - Bioenergetics, 2021, 1862, 148446.	0.5	30
141	Protein nanowires with tunable functionality and programmable self-assembly using sequence-controlled synthesis. Nature Communications, 2022, 13, 829.	5.8	30
142	Ultrafast Vibrational Frequency Shifts Induced by Electronic Excitations: Naphthols in Low Dielectric Media. Journal of Physical Chemistry A, 2012, 116, 2775-2790.	1.1	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.	1.5	29
144	Exploring Allosteric Pathways of a V-Type Enzyme with Dynamical Perturbation Networks. Journal of Physical Chemistry B, 2019, 123, 3452-3461.	1.2	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.	2.4	29
146	High-Potential Porphyrins Supported on SnO₂ and TiO₂ Surfaces for Photoelectrochemical Applications. Journal of Physical Chemistry C, 2016, 120, 28971-28982.	1.5	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.	5.5	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.	4.7	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.	3.3	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.	2.3	27
151	Behavior of Ruâ€“bda Waterâ€Oxidation Catalysts in Low Oxidation States. Chemistry - A European Journal, 2018, 24, 12838-12847.	1.7	27
152	Enhanced specificity mutations perturb allosteric signaling in CRISPR-Cas9. ELife, 2021, 10, .	2.8	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.	1.0	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.	1.1	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.	8.2	25
156	Vibrational Stark shift spectroscopy of catalysts under the influence of electric fields at electrodeâ€“solution interfaces. Chemical Science, 2021, 12, 10131-10149.	3.7	25
157	Ultrafast Solventâ€Assisted Electronic Level Crossing in 1â€Naphthol. Angewandte Chemie - International Edition, 2013, 52, 6871-6875.	7.2	24
158	Formate to Oxalate: A Crucial Step for the Conversion of Carbon Dioxide into Multiâ€carbon Compounds. ChemCatChem, 2016, 8, 3453-3457.	1.8	24
159	Tripletâ€“triplet energy transfer in artificial and natural photosynthetic antennas. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5513-E5521.	3.3	24
160	High-Energy Charge-Separated States by Reductive Electron Transfer Followed by Electron Shift in the Tetraphenylethyleneâ€“Aluminum(III) Porphyrinâ€“Fullerene Triad. Journal of Physical Chemistry C, 2019, 123, 131-143.	1.5	24
161	Fabrication of Modularly Functionalizable Microcapsules Using Protein-Based Technologies. ACS Biomaterials Science and Engineering, 2016, 2, 1856-1861.	2.6	23
162	Electronâ€“Hole-Pair-Induced Vibrational Energy Relaxation of Rhenium Catalysts on Gold Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 406-412.	2.1	22

#	Article	IF	Citations
163	Molecular design of light-harvesting photosensitizers: effect of varied linker conjugation on interfacial electron transfer. Physical Chemistry Chemical Physics, 2016, 18, 18678-18682.	1.3	21
164	Thermodynamics of the S₂-to-S₃ state transition of the oxygen-evolving complex of photosystem II. Physical Chemistry Chemical Physics, 2019, 21, 20840-20848.	1.3	21
165	Is Deprotonation of the Oxygen-Evolving Complex of Photosystem II during the S₁ â†' S₂ Transition Suppressed by Proton Quantum Delocalization?. Journal of the American Chemical Society, 2021, 143, 8324-8332.	6.6	21
166	Linker Rectifiers for Covalent Attachment of Transitionâ€Metal Catalysts to Metalâ€Oxide Surfaces. ChemPhysChem, 2014, 15, 1138-1147.	1.0	20
167	Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. Journal of Physical Chemistry A, 2016, 120, 3260-3269.	1.1	20
168	Thousandfold Enhancement of Photoreduction Lifetime in Re(bpy)(CO)₃ via Spin-Dependent Electron Transfer from a Perylenediimide Radical Anion Donor. Journal of the American Chemical Society, 2017, 139, 16466-16469.	6.6	20
169	Charge Transport and Rectification in Donorâ€“Acceptor Dyads. Journal of Physical Chemistry C, 2017, 121, 19053-19062.	1.5	20
170	Chiral Inversion of Amino Acids in Antiparallel Î²-Sheets at Interfaces Probed by Vibrational Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry B, 2019, 123, 5769-5781.	1.2	20
171	Regulation of MIF Enzymatic Activity by an Allosteric Site at the Central Solvent Channel. Cell Chemical Biology, 2020, 27, 740-750.e5.	2.5	20
172	Reply to Turin et al.: Vibrational theory of olfaction is implausible. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3155.	3.3	19
173	Beyond Local Group Modes in Vibrational Sum Frequency Generation. Journal of Physical Chemistry A, 2015, 119, 3407-3414.	1.1	18
174	Characterization of Protein Tyrosine Phosphatase 1B Inhibition by Chlorogenic Acid and Cichoric Acid. Biochemistry, 2017, 56, 96-106.	1.2	18
175	D1-S169A Substitution of Photosystem II Perturbs Water Oxidation. Biochemistry, 2019, 58, 1379-1387.	1.2	18
176	Relative stability of the S2 isomers of the oxygen evolving complex of photosystem II. Photosynthesis Research, 2019, 141, 331-341.	1.6	18
177	The Effect of (â^')-Epigallocatechin-3-Gallate on the Amyloid-Î² Secondary Structure. Biophysical Journal, 2020, 119, 349-359.	0.2	18
178	New Insights from Sum Frequency Generation Vibrational Spectroscopy into the Interactions of Islet Amyloid Polypeptides with Lipid Membranes. Journal of Diabetes Research, 2016, 2016, 1-17.	1.0	17
179	Assessment of DFT for Computing Sum Frequency Generation Spectra of an Epoxydiol and a Deuterated Isotopologue at Fused Silica/Vapor Interfaces. Journal of Physical Chemistry B, 2016, 120, 1919-1927.	1.2	17
180	Collaboration between experiment and theory in solar fuels research. Chemical Society Reviews, 2019, 48, 1865-1873.	18.7	17

#	Article	IF	Citations
181	The MP/SOFT methodology for simulations of quantum dynamics: Model study of the photoisomerization of the retinyl chromophore in visual rhodopsin. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 274-282.	2.0	16
182	MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the Oxytricha nova G-Quadruplex. Journal of Chemical Theory and Computation, 2014, 10, 5125-5135.	2.3	16
183	Insights into Photosystem II from Isomorphous Difference Fourier Maps of Femtosecond X-ray Diffraction Data and Quantum Mechanics/Molecular Mechanics Structural Models. ACS Energy Letters, 2017, 2, 397-407.	8.8	16
184	Inclusion of nuclear quantum effects for simulations of nonlinear spectroscopy. Journal of Chemical Physics, 2018, 148, 244105.	1.2	16
185	A conductive metalâ€“organic framework photoanode. Chemical Science, 2020, 11, 9593-9603.	3.7	16
186	The Oâ€“H Stretching Mode of a Prototypical Photoacid as a Local Dielectric Probe. Journal of Physical Chemistry A, 2011, 115, 10511-10516.	1.1	15
187	Triplet Oxygen Evolution Catalyzed by a Biomimetic Oxomanganese Complex: Functional Role of the Carboxylate Buffer. ACS Catalysis, 2015, 5, 2384-2390.	5.5	15
188	Vibronic Effects in the Ultrafast Interfacial Electron Transfer of Perylene-Sensitized TiO₂ Surfaces. Journal of Physical Chemistry C, 2019, 123, 12599-12607.	1.5	15
189	Water Network Dynamics Next to the Oxygen-Evolving Complex of Photosystem II. Inorganics, 2019, 7, 39.	1.2	15
190	Community Network Analysis of Allosteric Proteins. Methods in Molecular Biology, 2021, 2253, 137-151.	0.4	15
191	Electrochemical Reduction of Aqueous Imidazolium on Pt(111) by Proton Coupled Electron Transfer. Topics in Catalysis, 2015, 58, 23-29.	1.3	14
192	Preparation of Halogenated Fluorescent Diaminophenazine Building Blocks. Journal of Organic Chemistry, 2015, 80, 9881-9888.	1.7	14
193	Hot Hole Hopping in a Polyoxotitanate Cluster Terminated with Catechol Electron Donors. Journal of Physical Chemistry C, 2016, 120, 20006-20015.	1.5	14
194	Ammonia Binding in the Second Coordination Sphere of the Oxygen-Evolving Complex of Photosystem II. Biochemistry, 2016, 55, 4432-4436.	1.2	14
195	Unanticipated Stickiness of Î±-Pinene. Journal of Physical Chemistry A, 2017, 121, 3239-3246.	1.1	14
196	X-ray Free Electron Laser Radiation Damage through the S-State Cycle of the Oxygen-Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2017, 121, 9382-9388.	1.2	14
197	Multi-time formulation of Matsubara dynamics. Journal of Chemical Physics, 2019, 151, 034108.	1.2	14
198	Linker Length-Dependent Electron-Injection Dynamics of Trimesitylporphyrins on SnO₂ Films. Journal of Physical Chemistry C, 2017, 121, 22690-22699.	1.5	13

#	Article	IF	Citations
199	Inverse Design of a Catalyst for Aqueous CO/CO₂ Conversion Informed by the Ni^{II}â€“Iminothiolate Complex. Inorganic Chemistry, 2018, 57, 15474-15480.	1.9	13
200	Hammett neural networks: prediction of frontier orbital energies of tungstenâ€“benzylidyne photoredox complexes. Chemical Science, 2019, 10, 6844-6854.	3.7	13
201	High-Conductance Conformers in Histograms of Single-Molecule Currentâ€“Voltage Characteristics. Journal of Physical Chemistry C, 2014, 118, 8316-8321.	1.5	12
202	Interfacial Electron Transfer Followed by Photooxidation in N,N-Bis(p-anisole)aminopyridineâ€“Aluminum(III) Porphyrinâ€“Titanium(IV) Oxide Self-Assembled Photoanodes. Journal of Physical Chemistry C, 2017, 121, 14484-14497.	1.5	12
203	Antimony Complexes for Electrocatalysis: Activity of a Mainâ€Group Element in Proton Reduction. Angewandte Chemie, 2017, 129, 9239-9243.	1.6	12
204	Characterization of ammonia binding to the second coordination shell of the oxygen-evolving complex of photosystem II. Dalton Transactions, 2017, 46, 16089-16095.	1.6	12
205	Mechanism of Inhibition of the Reproduction of SARS-CoV-2 and Ebola Viruses by Remdesivir. Biochemistry, 2021, 60, 1869-1875.	1.2	12
206	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. Biochemistry, 2022, 61, 785-794.	1.2	12
207	Ferroceneâ€Promoted Longâ€Cycle Lithiumâ€“Sulfur Batteries. Angewandte Chemie, 2016, 128, 15038-15042.	1.6	11
208	Ring-polymer, centroid, and mean-field approximations to multi-time Matsubara dynamics. Journal of Chemical Physics, 2020, 153, 124112.	1.2	11
209	Do crystallographic XFEL data support binding of a water molecule to the oxygen-evolving complex of photosystem II exposed to two flashes of light?. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11
210	Quantum Dynamics of the Excitedâ€State Intramolecular Proton Transfer in 2â€(2â€²â€Hydroxyphenyl)benzothiazole. Israel Journal of Chemistry, 2009, 49, 187-197.	1.0	10
211	Floquet Study of Quantum Control of the Cisâ€“Trans Photoisomerization of Rhodopsin. Journal of Chemical Theory and Computation, 2018, 14, 1198-1205.	2.3	10
212	Carbon chain shape selectivity by the mouse olfactory receptor OR-I7. Organic and Biomolecular Chemistry, 2018, 16, 2541-2548.	1.5	10
213	Dopant-Dependent SFG Response of Rhenium CO₂ Reduction Catalysts Chemisorbed on SrTiO₃ (100) Single Crystals. Journal of Physical Chemistry C, 2018, 122, 13944-13952.	1.5	10
214	Regioselective Ultrafast Photoinduced Electron Transfer from Naphthols to Halocarbon Solvents. Journal of Physical Chemistry Letters, 2019, 10, 2657-2662.	2.1	10
215	Effect of Electronic Coupling on Electron Transfer Rates from Photoexcited Naphthalenediimide Radical Anion to Re(bpy)(CO)₃X. Journal of Physical Chemistry C, 2019, 123, 10178-10190.	1.5	10
216	Atmospheric Î²-Caryophyllene-Derived Ozonolysis Products at Interfaces. ACS Earth and Space Chemistry, 2019, 3, 158-169.	1.2	10

#	Article	IF	Citations
217	Surprisingly big linker-dependence of activity and selectivity in CO₂ reduction by an iridium(<scp>i</scp>) pincer complex. Chemical Communications, 2020, 56, 9126-9129.	2.2	10
218	Computational insights into the membrane fusion mechanism of SARS-CoV-2 at the cellular level. Computational and Structural Biotechnology Journal, 2021, 19, 5019-5028.	1.9	10
219	Insights into Binding of Single-Stranded Viral RNA Template to the Replicationâ€“Transcription Complex of SARS-CoV-2 for the Priming Reaction from Molecular Dynamics Simulations. Biochemistry, 2022, 61, 424-432.	1.2	10
220	Functional Tensor-Train Chebyshev Method for Multidimensional Quantum Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 25-36.	2.3	10
221	Two-dimensional Raman spectroscopy of Lennard-Jones liquids via ring-polymer molecular dynamics. Journal of Chemical Physics, 2020, 153, 034117.	1.2	9
222	Tensor-Train Split-Operator KSL (TT-SOKSL) Method for Quantum Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 3327-3346.	2.3	9
223	Orientations of nonlocal vibrational modes from combined experimental and theoretical sum frequency spectroscopy. Chemical Physics Letters, 2017, 683, 199-204.	1.2	8
224	Ultrafast photo-induced charge transfer of 1-naphthol and 2-naphthol to halocarbon solvents. Chemical Physics Letters, 2017, 683, 49-56.	1.2	8
225	Distinct Binding of Rhenium Catalysts on Nanostructured and Single-Crystalline TiO₂ Surfaces Revealed by Two-Dimensional Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 26018-26031.	1.5	8
226	Iterative Power Algorithm for Global Optimization with Quantics Tensor Trains. Journal of Chemical Theory and Computation, 2021, 17, 3280-3291.	2.3	8
227	Heterogeneous Composition of Oxygen-Evolving Complexes in Crystal Structures of Dark-Adapted Photosystem II. Biochemistry, 2021, 60, 3374-3384.	1.2	8
228	Distinct allosteric pathways in imidazole glycerol phosphate synthase from yeast and bacteria. Biophysical Journal, 2022, 121, 119-130.	0.2	8
229	Semiclassical Molecular Dynamics Simulations of the Excited State Photodissociation Dynamics of H2O in the A1B1Bandâ€. Journal of Physical Chemistry B, 2002, 106, 8271-8277.	1.2	7
230	Structureâ€“function relationships in single molecule rectification by N-phenylbenzamide derivatives. New Journal of Chemistry, 2016, 40, 7373-7378.	1.4	7
231	Effects of aligned Î±â€helix peptide dipoles on experimental electrostatic potentials. Protein Science, 2017, 26, 1692-1697.	3.1	7
232	On the relationship between cumulative correlation coefficients and the quality of crystallographic data sets. Protein Science, 2017, 26, 2410-2416.	3.1	7
233	Thermodynamic and Structural Factors That Influence the Redox Potentials of Tungstenâ€“Alkylidyne Complexes. ACS Catalysis, 2017, 7, 6134-6143.	5.5	7
234	A Multispecific Investigation of the Metal Effect in Mammalian Odorant Receptors for Sulfur-Containing Compounds. Chemical Senses, 2018, 43, 357-366.	1.1	7

#	Article	IF	Citations
235	Robust Binding of Disulfide-Substituted Rhenium Bipyridyl Complexes for CO2 Reduction on Gold Electrodes. Frontiers in Chemistry, 2020, 8, 86.	1.8	7
236	A structurally preserved allosteric site in the MIF superfamily affects enzymatic activity and CD74 activation in D-dopachrome tautomerase. Journal of Biological Chemistry, 2021, 297, 101061.	1.6	7
237	MptpA Kinetics Enhanced by Allosteric Control of an Active Conformation. Journal of Molecular Biology, 2022, 434, 167540.	2.0	7
238	Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants. Journal of Chemical Physics, 2017, 146, 215104.	1.2	6
239	Semiconductor-to-conductor transition in 2D copper(<scp>ii</scp>) oxide nanosheets through surface sulfur-functionalization. Nanoscale, 2020, 12, 14549-14559.	2.8	6
240	Development of an Enantioselective Synthesis of (âˆ')-Euonyminol. Journal of Organic Chemistry, 2021, 86, 17011-17035.	1.7	6
241	Energy Flow Under Control. Science, 2009, 326, 245-246.	6.0	5
242	Ultraviolet vision: photophysical properties of the unprotonated retinyl Schiff base in the Siberian hamster cone pigment. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	5
243	Inferring Protonation States of Hydroxamate Adsorbates on TiO₂ Surfaces. Journal of Physical Chemistry C, 2017, 121, 11985-11990.	1.5	5
244	Ultrafast proton-assisted tunneling through ZrO₂ in dye-sensitized SnO₂-core/ZrO₂-shell films. Chemical Communications, 2018, 54, 7971-7974.	2.2	5
245	Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast Xâ€Ray Absorption Spectroscopy. Angewandte Chemie - International Edition, 2020, 59, 20044-20048.	7.2	5
246	Identification of a Na⁺-Binding Site near the Oxygen-Evolving Complex of Spinach Photosystem II. Biochemistry, 2020, 59, 2823-2831.	1.2	5
247	Allosteric Impact of the Variable Insert Loop in Vaccinia H1-Related (VHR) Phosphatase. Biochemistry, 2020, 59, 1896-1908.	1.2	5
248	Organometallic Iridium Complex Containing a Dianionic, Tridentate, Mixed Organicâ€“Inorganic Ligand. Inorganic Chemistry, 2016, 55, 8121-8129.	1.9	4
249	Classical Optimal Control for Energy Minimization Based On Diffeomorphic Modulation under Observable-Response-Preserving Homotopy. Journal of Chemical Theory and Computation, 2018, 14, 3351-3362.	2.3	4
250	D1-S169A substitution of photosystem II reveals a novel S2-state structure. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148301.	0.5	4
251	Selective Heterogeneous Transfer Hydrogenation from Tertiary Amines to Alkynes. ACS Catalysis, 2021, 11, 5405-5415.	5.5	4
252	Tuning the Conduction Band for Interfacial Electron Transfer: Dye-Sensitized Sn_xTi_{1â€“x}O₂ Photoanodes for Water Splitting. ACS Applied Energy Materials, 2021, 4, 4695-4703.	2.5	4

#	Article	IF	Citations
253	Chapter 1. Inverse molecular design for materials discovery. Chemical Modelling, 2013, , 1-31.	0.2	4
254	Binding of the substrate analog methanol in the oxygen-evolving complex of photosystem II in the D1-N87A genetic variant of cyanobacteria. Faraday Discussions, 2022, 234, 195-213.	1.6	4
255	Multiple unitary-pulses for coherent-control of tunnelling and decoherence. Journal of Modern Optics, 2007, 54, 2617-2627.	0.6	3
256	Tunneling through Coulombic barriers: quantum control of nuclear fusion. Molecular Physics, 2012, 110, 995-999.	0.8	3
257	Kepler Predictorâ€“Corrector Algorithm: Scattering Dynamics with One-Over-R Singular Potentials. Journal of Chemical Theory and Computation, 2012, 8, 24-35.	2.3	3
258	Steered Quantum Dynamics for Energy Minimization. Journal of Physical Chemistry B, 2015, 119, 715-727.	1.2	3
259	Facile solvolysis of a surprisingly twisted tertiary amide. New Journal of Chemistry, 2016, 40, 1974-1981.	1.4	3
260	Reduced Occupancy of the Oxygen-Evolving Complex of Photosystem II Detected in Cryo-Electron Microscopy Maps. Biochemistry, 2018, 57, 5925-5929.	1.2	3
261	Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast Xâ€Ray Absorption Spectroscopy. Angewandte Chemie, 2020, 132, 20219-20223.	1.6	3
262	Allosteric Control of Enzyme Activity: From Ancient Origins to Recent Gene-Editing Technologies. Biochemistry, 2020, 59, 1711-1712.	1.2	3
263	Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry B, 2017, 121, 11425-11426.	1.2	2
264	Mechanistic study of CO/CO 2 conversion catalyzed by a biomimetic Ni(II)â€iminothiolate complex. International Journal of Quantum Chemistry, 2018, 118, e25555.	1.0	2
265	Nanosecond Dynamics Regulate the MIFâ€Induced Activity of CD74. Angewandte Chemie, 2018, 130, 7234-7237.	1.6	2
266	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
267	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2
268	Computational Studies of the Oxygen-Evolving Complex of Photosystem II and Biomimetic Oxomanganese Complexes for Renewable Energy Applications. ACS Symposium Series, 2013, , 203-215.	0.5	1
269	Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry A, 2017, 121, 9680-9681.	1.1	1
270	Is the Supporting Information the Venue for Reproducibility and Transparency?. Journal of Physical Chemistry C, 2017, 121, 28212-28213.	1.5	1

#	Article	IF	Citations
271	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
272	The JPC Periodic Table. Journal of Physical Chemistry C, 2019, 123, 17063-17074.	1.5	1
273	Distorted Copper(II) Complex with Unusually Short CFÂ·Â·Â·Cu Distances. Inorganic Chemistry, 2021, 60, 14759-14764.	1.9	1
274	Glycerol binding at the narrow channel of photosystem II stabilizes the low-spin S2 state of the oxygen-evolving complex. Photosynthesis Research, 2022, , 1.	1.6	1
275	InnenrÃ¼cktitelbild: Ultrafast Solvent-Assisted Electronic Level Crossing in 1-Naphthol (Angew. Chem.) Tj ETQq1 1 0.784314 rgBT /O	1.6	0
276	Introducing special issue on photocatalysis and photoelectrochemistry. Journal of Chemical Physics, 2021, 154, 190401.	1.2	0