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List of Publications by Year in descending order

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69
papers

2,806
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236925

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all docs

73
docs citations

73
times ranked

2735
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantum Mechanics/Molecular Mechanics Study of the Catalytic Cycle of Water Splitting in Photosystem II. <i>Journal of the American Chemical Society</i> , 2008, 130, 3428-3442.	13.7	345
2	Interplay of Charge State, Lability, and Magnetism in the Molecule-like Au ₂₅ (SR) ₁₈ Cluster. <i>Journal of the American Chemical Society</i> , 2013, 135, 15585-15594.	13.7	203
3	Computational studies of the O ₂ -evolving complex of photosystem II and biomimetic oxomanganese complexes. <i>Coordination Chemistry Reviews</i> , 2008, 252, 395-415.	18.8	146
4	Au ₂₅ (SET) ₁₈ , a Nearly Naked Thiolate-Protected Au ₂₅ Cluster: Structural Analysis by Single Crystal X-ray Crystallography and Electron Nuclear Double Resonance. <i>ACS Nano</i> , 2014, 8, 3904-3912.	14.6	145
5	QM/MM Models of the O ₂ -Evolving Complex of Photosystem II. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1119-1134.	5.3	136
6	Effect of the Charge State ($\langle i \rangle z \langle i \rangle = \hat{a}^{-1} 1, 0, +1$) on the Nuclear Magnetic Resonance of Monodisperse Au ₂₅ [S(CH ₂) ₂] ₂ Ph ₁₈ Clusters. <i>Analytical Chemistry</i> , 2011, 83, 6355-6362.	6.5	124
7	The mechanism of photosynthetic water splitting. <i>Photochemical and Photobiological Sciences</i> , 2005, 4, 940.	2.9	111
8	A Model of the Oxygen-Evolving Center of Photosystem II Predicted by Structural Refinement Based on EXAFS Simulations. <i>Journal of the American Chemical Society</i> , 2008, 130, 6728-6730.	13.7	110
9	Characterization of synthetic oxomanganese complexes and the inorganic core of the O ₂ -evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 786-800.	3.5	99
10	QM/MM Study of Energy Storage and Molecular Rearrangements Due to the Primary Event in Vision. <i>Biophysical Journal</i> , 2004, 87, 2931-2941.	0.5	98
11	Quantum mechanics/molecular mechanics structural models of the oxygen-evolving complex of photosystem II. <i>Current Opinion in Structural Biology</i> , 2007, 17, 173-180.	5.7	91
12	QM/MM Approaches in Medicinal Chemistry Research. <i>Current Topics in Medicinal Chemistry</i> , 2010, 10, 46-54.	2.1	83
13	Proof for the Concerted Inversion Mechanism in the $\langle i \rangle \text{trans} \langle i \rangle \hat{a}^{-1} \langle i \rangle \text{cis} \langle i \rangle$ Isomerization of Azobenzene Using Hydrogen Bonding To Induce Isomer Locking. <i>Journal of Organic Chemistry</i> , 2010, 75, 4817-4827.	3.2	79
14	Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. <i>Accounts of Chemical Research</i> , 2006, 39, 184-193.	15.6	75
15	QM/MM computational studies of substrate water binding to the oxygen-evolving centre of photosystem II. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2008, 363, 1149-1156.	4.0	70
16	Computational insights into the O ₂ -evolving complex of photosystem II. <i>Photosynthesis Research</i> , 2008, 97, 91-114.	2.9	62
17	A Self-Consistent Space-Domain Decomposition Method for QM/MM Computations of Protein Electrostatic Potentials. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 175-186.	5.3	47
18	QM/MM Study of the NMR Spectroscopy of the Retinyl Chromophore in Visual Rhodopsin. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 674-685.	5.3	45

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19	Synthesis and structure-activity relationships of metal-ligand complexes that potently inhibit cell migration. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 498-504.	2.2	45
20	The MoD-QM/MM methodology for structural refinement of photosystem II and other biological macromolecules. <i>Photosynthesis Research</i> , 2009, 102, 455-470.	2.9	41
21	Handedness Enantioselection of Carbon Nanotubes Using Helical Assemblies of Flavin Mononucleotide. <i>Journal of the American Chemical Society</i> , 2012, 134, 13196-13199.	13.7	40
22	A magnetic look into the protecting layer of Au ₂₅ clusters. <i>Chemical Science</i> , 2016, 7, 6910-6918.	7.4	33
23	QM/MM investigation of structure and spectroscopic properties of a vanadium-containing peroxidase. <i>Journal of Inorganic Biochemistry</i> , 2008, 102, 1684-1690.	3.5	32
24	Bacteriochlorins with a Twist: Discovery of a Unique Mechanism to Red-Shift the Optical Spectra of Bacteriochlorins. <i>Journal of the American Chemical Society</i> , 2017, 139, 548-560.	13.7	32
25	Atomically precise Au ₁₄₄ (SR) ₆₀ nanoclusters (R = Et, Pr) are capped by 12 distinct ligand types of 5-fold equivalence and display gigantic diastereotopic effects. <i>Chemical Science</i> , 2018, 9, 8796-8805.	7.4	30
26	Dual Modifications of Î±-Galactosylceramide Synergize to Promote Activation of Human Invariant Natural Killer T Cells and Stimulate Anti-tumor Immunity. <i>Cell Chemical Biology</i> , 2018, 25, 571-584.e8.	5.2	27
27	Atomistic Prediction of Sorption Free Energies of Cationic Aromatic Amines on Montmorillonite: A Linear Interaction Energy Method. <i>Environmental Science and Technology Letters</i> , 2014, 1, 284-289.	8.7	24
28	Thermodynamics of the Quasi-Epitaxial Flavin Assembly around Various-Chirality Carbon Nanotubes. <i>Journal of the American Chemical Society</i> , 2014, 136, 7452-7463.	13.7	23
29	Bacterio- and Isobacteriodilactones by Stepwise or Direct Oxidations of <i>meso</i> -Tetrakis(pentafluorophenyl)porphyrin. <i>Journal of Organic Chemistry</i> , 2019, 84, 239-256.	3.2	23
30	Stability of <i>N</i> -Glycosidic Bond of (5 <i>S</i>)-8,5'-Cyclo-2'-deoxyguanosine. <i>Chemical Research in Toxicology</i> , 2012, 25, 2451-2461.	3.3	21
31	Locostatin Disrupts Association of Raf Kinase Inhibitor Protein With Binding Proteins by Modifying a Conserved Histidine Residue in the Ligand-Binding Pocket. <i>Forum on Immunopathological Diseases and Therapeutics</i> , 2011, 2, 47-58.	0.1	21
32	Vibrational Coupling Modulation in <i>n</i> -Alkanethiolate Protected Au ₂₅ (SR) ₁₈ Clusters. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25378-25386.	3.1	20
33	Preparation of Some Homologous TEMPO Nitroxides and Oxoammonium Salts; Notes on the NMR Spectroscopy of Nitroxide Free Radicals; Observed Radical Nature of Oxoammonium Salt Solutions Containing Trace Amounts of Corresponding Nitroxides in an Equilibrium Relationship. <i>Journal of Organic Chemistry</i> , 2017, 82, 9279-9290.	3.2	19
34	Computational and experimental investigations of mono-septanoside binding by Concanavalin A: correlation of ligand stereochemistry to enthalpies of binding. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 154-164.	2.8	18
35	Chromene-Annulated Bacteriochlorins. <i>Journal of Organic Chemistry</i> , 2016, 81, 3603-3618.	3.2	18
36	QM/MM Prediction of the Stark Shift in the Active Site of a Protein. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2817-2823.	5.3	17

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37	Site-Preferential Dissociation of Peptides with Active Chemical Modification for Improving Fragment Ion Detection. <i>Analytical Chemistry</i> , 2010, 82, 23-27.	6.5	16
38	MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the <i>Oxytricha nova</i> G-Quadruplex. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5125-5135.	5.3	16
39	Optimization of cutting schemes for the evaluation of molecular electrostatic potentials in proteins via Moving-Domain QM/MM. <i>Journal of Molecular Modeling</i> , 2008, 14, 1-9.	1.8	15
40	Fullerene-Assisted Photoinduced Charge Transfer of Single-Walled Carbon Nanotubes through a Flavin Helix. <i>Journal of the American Chemical Society</i> , 2016, 138, 5904-5915.	13.7	15
41	Origins of the Electronic Modulations of Bacterio- and Isobacteriodilactone Regioisomers. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7470-7485.	2.5	14
42	Unexpected Cleavage of 2-Azido-2-(hydroxymethyl)oxetanes: Conformation Determines Reaction Pathway?. <i>Journal of Organic Chemistry</i> , 2010, 75, 7565-7572.	3.2	13
43	Recognition and Reactivity in the Binding between Raf Kinase Inhibitor Protein and Its Small-Molecule Inhibitor Locostatin. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10176-10181.	2.6	12
44	A QM/MM approach for the study of monolayer-protected gold clusters. <i>Journal of Materials Science</i> , 2012, 47, 7686-7692.	3.7	12
45	Spectral Signatures of Canthaxanthin Translocation in the Orange Carotenoid Protein. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11387-11395.	2.6	12
46	Molecular Modeling Characterization of a Conformationally Constrained Monolayer-Protected Gold Cluster. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16043-16050.	3.1	11
47	Short-Circuiting Azobenzene Photoisomerization with Electron-Donating Substituents and Reactivating the Photochemistry with Chemical Modification. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 2916-2919.	2.4	10
48	Connectivity-Based Biocompatible Force Field for Thiolated Gold Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27804-27812.	3.1	10
49	Fluorescence Anisotropy Detection of Barrier Crossing and Ultrafast Conformational Dynamics in the S ₂ State of β -Carotene. <i>Journal of Physical Chemistry B</i> , 2020, 124, 9029-9046.	2.6	10
50	Silicon Acceleration of a Tandem Alkene Isomerization/Electrocyclic Ring-opening of 2-Methyleneoxetanes to α,β -Unsaturated Methylketones. <i>Journal of Organic Chemistry</i> , 2013, 78, 11213-11220.	3.2	9
51	Light Harvesting by Equally Contributing Mechanisms in a Photosynthetic Antenna Protein. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 563-568.	4.6	8
52	Carotenoid-Chlorophyll Interactions in a Photosynthetic Antenna Protein: A Supramolecular QM/MM Approach. <i>Molecules</i> , 2018, 23, 2589.	3.8	7
53	Interexciton nonradiative relaxation pathways in the peridinin-chlorophyll protein. <i>Cell Reports Physical Science</i> , 2021, 2, 100380.	5.6	7
54	Formation of and Glycosylation with Peracetyl Septanosyl Halides: Rationalizing Complex Reactivity En Route to <i>p</i> -Nitrophenyl Septanosides. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 1709-1719.	2.4	6

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55	Aluminosilicate Mineralogy and the Sorption of Organic Cations: Interplay between Electrostatic Barriers and Compound Structural Features. <i>Environmental Science & Technology</i> , 2020, 54, 1623-1633.	10.0	6
56	Protein polarization effects in the thermodynamic computation of vibrational Stark shifts. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	6
57	Amide-Linked C4â€³-Saccharide Modification of KRN7000 Provides Potent Stimulation of Human Invariant NKT Cells and Anti-Tumor Immunity in a Humanized Mouse Model. <i>ACS Chemical Biology</i> , 2020, 15, 3176-3186.	3.4	6
58	The MOD-QM/MM Method. <i>Methods in Enzymology</i> , 2016, 577, 443-481.	1.0	4
59	The limited extent of the electronic modulation of chlorins and bacteriochlorins through chromene-annulation. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18233-18240.	2.8	4
60	High-Throughput Non-targeted Chemical Structure Identification Using Gas-Phase Infrared Spectra. <i>Analytical Chemistry</i> , 2021, 93, 10688-10696.	6.5	4
61	Electronic energy levels of porphyrins are influenced by the local chemical environment. <i>RSC Advances</i> , 2022, 12, 1361-1365.	3.6	4
62	Interaction of H₂@C₆₀ and Nitroxide through Conformationally Constrained Peptide Bridges. <i>Photochemistry and Photobiology</i> , 2014, 90, 439-447.	2.5	3
63	A favorable path to domain separation in the orange carotenoid protein. <i>Protein Science</i> , 2022, 31, 850-863.	7.6	3
64	SURFACE EFFECTS ON THE STATISTICS OF THE LOCAL DENSITY OF STATES IN METALLIC NANOPARTICLES: MANIFESTATION ON THE NMR SPECTRA. <i>Modern Physics Letters B</i> , 2005, 19, 1285-1294.	1.9	2
65	Spectral Features of Canthaxanthin in HCP2. A QM/MM Approach. <i>Molecules</i> , 2021, 26, 2441.	3.8	2
66	Easily accessible non-aromatic heterocycles with handles: 4-bromo-2,3-dihydrofurans from 1,2-dibromohomoallylic alcohols. <i>Chemical Science</i> , 2021, 12, 10347-10353.	7.4	2
67	Ligation Of The C-Terminus Of The D1 Polypeptide Of Photosystem Ii To The Oxygen Evolving Complex: A Dft-Qm/Mm Study. , 2008, , 363-368.		2
68	An extrapolation method for computing protein solvation energies based on density fragmentation of a graphical surface tessellation. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 30, 38-45.	2.4	1
69	Insights into diastereotopic effects in thiolated gold nanoclusters. <i>Chemical Physics Letters</i> , 2021, 770, 138448.	2.6	1