Jun-ya Hasegawa

List of Publications by Year
in descending order

129 papers	4,930 citations	126907 33 h-index	102487 66 g-index
137 all docs	137 docs citations	137 times ranked	4955 citing authors

#	Article	IF	Citations
1	Câ€“H Bond Activation Mechanism by a Pd(II)â€“(Î¼-O)â€“Au(0) Structure Unique to Heterogeneous Catalysts. Jacs Au, 2022, 2, 394-406.	7.9	6
2	Photoinduced Copper-Catalyzed Asymmetric Acylation of Allylic Phosphates with Acylsilanes. Journal of the American Chemical Society, 2022, 144, 2218-2224.	13.7	39
3	Deoxygenative CO₂ conversions with triphenylborane and phenylsilane in the presence of secondary amines or nitrogen-containing aromatics. Green Chemistry, 2022, 24, 2385-2390.	9.0	12
4	Doubly linked chiral phenanthrene oligomers for homogeneously Ï€-extended helicenes with large effective conjugation length. Nature Communications, 2022, 13, 1475.	12.8	24
5	Exploring the Reaction Mechanism of Heterobimetallic Nickelâ€Alkali Catalysts for Ethylene Polymerization: Secondaryâ€Metalâ€Ligand Cooperative Catalysis. ChemCatChem, 2022, 14, .	3.7	5
6	Reaction Mechanism of Deoxydehydration by Ceria-Supported Monomeric Rhenium Catalysts: A Computational Study. Journal of Physical Chemistry C, 2022, 126, 11566-11573.	3.1	6
7	Chemoselective Transesterification of Methyl (Meth)acrylates Catalyzed by Sodium(I) or Magnesium(II) Aryloxides. ACS Catalysis, 2021, 11, 199-207.	11.2	10
8	Mechanistic study of Câ€“H bond activation by O₂ on negatively charged Au clusters: Î±,Î²-dehydrogenation of 1-methyl-4-piperidone by supported Au catalysts. Catalysis Science and Technology, 2021, 11, 3333-3346.	4.1	5
9	Design and prediction of high potentansa-zirconocene catalyst for olefin polymerizations: combined DFT calculations and QSPR approach. New Journal of Chemistry, 2021, 45, 8248-8257.	2.8	5
10	Impact of tensile and compressive forces on the hydrolysis of cellulose and chitin. Physical Chemistry Chemical Physics, 2021, 23, 15908-15916.	2.8	15
11	Tuning Transition Electric and Magnetic Dipole Moments: [7]Helicenes Showing Intense Circularly Polarized Luminescence. Journal of Physical Chemistry Letters, 2021, 12, 686-695.	4.6	107
12	A Triad Fluorenone Derivative Bearing Two Imidazole Groups That Switches between Three States by Base and Acid Stimuli. Chemistry Letters, 2021, 50, 1363-1367.	1.3	0
13	Co Single Atoms in ZrO₂ with Inherent Oxygen Vacancies for Selective Hydrogenation of CO₂ to CO. ACS Catalysis, 2021, 11, 9450-9461.	11.2	116
14	On the Electronic Structure Origin of Mechanochemically Induced Selectivity in Acid-Catalyzed Chitin Hydrolysis. Journal of Physical Chemistry A, 2021, 125, 187-197.	2.5	13
15	OpenMechanochem: A Python module for mechanochemical simulations. SoftwareX, 2021, 16, 100879.	2.6	1
16	Extending nudged elastic band method to reaction pathways involving multiple spin states. Journal of Chemical Physics, 2020, 153, 134114.	3.0	4
17	Catalytic Mechanism of Liquid-Metal Indium for Direct Dehydrogenative Conversion of Methane to Higher Hydrocarbons. ACS Omega, 2020, 5, 28158-28167.	3.5	15
18	Mechanistic Study on Deoxydehydration and Hydrogenation of Methyl Glycosides to Dideoxy Sugars over a ReO_xâ€“Pd/CeO₂ Catalyst. ACS Catalysis, 2020, 10, 12040-12051.	11.2	21

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19	Spinâ€inversion mechanisms in O 2 binding to a model heme compound: A perspective from nonadiabatic wave packet calculations. Journal of Computational Chemistry, 2020, 41, 2527-2537.	3.3	2
20	Self-Assembled Multilayer Iron(0) Nanoparticle Catalyst for Ligand-Free Carbonâ€“Carbon/Carbonâ€“Nitrogen Bond-Forming Reactions. Organic Letters, 2020, 22, 7244-7249.	4.6	18
21	Aluminum porphyrins with quaternary ammonium halides as catalysts for copolymerization of cyclohexene oxide and CO₂: metalâ€“ligand cooperative catalysis. Chemical Science, 2020, 11, 5669-5675.	7.4	54
22	Delocalization Effect Promoted the Indoor Air Purification via Directly Unlocking the Ring-Opening Pathway of Toluene. Environmental Science & Technology, 2020, 54, 9693-9701.	10.0	63
23	Roles of Salicylate Donors in Enhancement of Productivity and Isotacticity of Zieglerâ€“Natta Catalyzed Propylene Polymerization. Polymers, 2020, 12, 883.	4.5	6
24	Synthesis of silyl formates, formamides, and aldehydes via solvent-free organocatalytic hydrosilylation of CO2. Chemical Communications, 2020, 56, 5783-5786.	4.1	37
25	Spinâ€inversion mechanisms in O 2 binding to a model heme complex revisited by density function theory calculations. Journal of Computational Chemistry, 2020, 41, 1130-1138.	3.3	12
26	Selective Catalytic Reduction of NO_x with NH₃ by Using Novel Catalysts: State of the Art and Future Prospects. Chemical Reviews, 2019, 119, 10916-10976.	47.7	1,003
27	Methylâ€Selective Î±â€Oxygenation of Tertiary Amines to Formamides by Employing Copper/Moderately Hindered Nitroxyl Radical (DMNâ€AZADO or 1â€Meâ€AZADO). Angewandte Chemie - International Edition, 2019, 58, 16651-16659.	13.8	19
28	Electrostatic Stabilization of Single-Atom Catalysts by Ionic Liquids. CheM, 2019, 5, 3207-3219.	11.7	131
29	Theoretical Study on the Câ€“H Activation of Methane by Liquid Metal Indium: Catalytic Activity of Small Indium Clusters. Journal of Physical Chemistry A, 2019, 123, 8907-8912.	2.5	16
30	Ni-Catalyzed Cycloisomerization between 3-Phenoxy Acrylic Acid Derivatives and Alkynes via Intramolecular Cleavage and Formation of the Câ€“O Bond To Give 2,3-Disubstituted Benzofurans. Organic Letters, 2019, 21, 8400-8403.	4.6	25
31	Adsorption mediated tandem acid catalyzed cellulose hydrolysis by ortho-substituted benzoic acids. Molecular Catalysis, 2019, 475, 110459.	2.0	6
32	Selective Synthesis of Primary Anilines from NH₃ and Cyclohexanones by Utilizing Preferential Adsorption of Styrene on the Pd Nanoparticle Surface. Angewandte Chemie - International Edition, 2019, 58, 10893-10897.	13.8	40
33	Theoretical Study on the Rhodium-Catalyzed Hydrosilylation of Câ•C and Câ•O Double Bonds with Tertiary Silane. Journal of Organic Chemistry, 2019, 84, 8552-8561.	3.2	17
34	SO₂-Tolerant Selective Catalytic Reduction of NO_x over Meso-TiO₂@Fe₂O₃@Al₂O₃ Metal-Based Monolith Catalysts. Environmental Science & Technology, 2019, 53, 6462-6473.	10.0	171
35	Experimental and theoretical study of multinuclear indiumâ€“oxo clusters in CHA zeolite for CH₄ activation at room temperature. Physical Chemistry Chemical Physics, 2019, 21, 13415-13427.	2.8	18
36	DFT Mechanistic Study on the Complete Oxidation of Ethylene by the Silica-Supported Pt Catalyst: Câ•C Activation via the Ethylene Dioxide Intermediate. Journal of Physical Chemistry C, 2019, 123, 12706-12715.	3.1	19

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37	<scp>l</scp>-Cysteine-Modified Acacia Gum as a Multifunctional Binder for Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2019, 11, 47956-47962.	8.0	16
38	Constraint structure optimization to a specific minimum using ionization energy. Journal of Computational Chemistry, 2019, 40, 507-514.	3.3	1
39	Excited States and Electron-transfer in Bacterial Photosynthetic Reaction Center: SAC-CI Theoretical Study. , 2019, , 790-793.		0
40	Quaternary Alkyl Ammonium Salt-Catalyzed Transformation of Glycidol to Glycidyl Esters by Transesterification of Methyl Esters. ACS Catalysis, 2018, 8, 1097-1103.	11.2	21
41	Transition States of Spin-State Crossing Reactions from Organometallics to Biomolecular Excited States. , 2018, , 289-313.		0
42	CuCl/TMEDA/nor-AZADO-catalyzed aerobic oxidative acylation of amides with alcohols to produce imides. Chemical Science, 2018, 9, 4756-4768.	7.4	34
43	First-Order Interacting Space Approach to Excited-State Molecular Interaction: Solvatochromic Shift of p-Coumaric Acid and Retinal Schiff Base. Journal of Chemical Theory and Computation, 2018, 14, 3643-3655.	5.3	3
44	Hidden radical reactivity of the [FeO]2+ group in the H-abstraction from methane: DFT and CASPT2 supported mechanism by the example of model iron (hydro)oxide species. Chemical Physics Letters, 2017, 679, 193-199.	2.6	10
45	A coordination strategy to realize a sextuply-bonded complex. Physical Chemistry Chemical Physics, 2017, 19, 14947-14954.	2.8	8
46	Selective Dehydration of Mannitol to Isomannide over HÎ² Zeolite. ACS Catalysis, 2017, 7, 4828-4834.	11.2	26
47	Selected configuration interaction method using sampled first-order corrections to wave functions. Journal of Chemical Physics, 2017, 147, 034102.	3.0	27
48	Formation of a New, Strongly Basic Nitrogen Anion by Metal Oxide Modification. Journal of the American Chemical Society, 2017, 139, 11857-11867.	13.7	27
49	Catalytic Cyclopropanation by Myoglobin Reconstituted with Iron Porphycene: Acceleration of Catalysis due to Rapid Formation of the Carbene Species. Journal of the American Chemical Society, 2017, 139, 17265-17268.	13.7	110
50	Recyclable and efficient polyurethane-Ir catalysts for direct borylation of aromatic compounds. Polymer Chemistry, 2017, 8, 7406-7415.	3.9	5
51	Photo-induced Î²-elimination of 9-fluorenylmethanol leading to dibenzofulvene. Chemical Communications, 2017, 53, 8431-8434.	4.1	2
52	Theoretical Study on Highly Active Bifunctional Metalloporphyrin Catalysts for the Coupling Reaction of Epoxides with Carbon Dioxide. Chemical Record, 2016, 16, 2260-2267.	5.8	29
53	Frontispiece: Highly Active and Robust Metalloporphyrin Catalysts for the Synthesis of Cyclic Carbonates from a Broad Range of Epoxides and Carbon Dioxide. Chemistry - A European Journal, 2016, 22, .	3.3	0
54	Electronic Polarization Effect of the Water Environment in Charge-Separated Donorâ€“Acceptor Systems: An Effective Fragment Potential Model Study. Journal of Physical Chemistry A, 2016, 120, 10273-10280.	2.5	0

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55	Spin-Blocking Effect in CO and H₂ Binding Reactions to Molybdenocene and Tungstenocene: A Theoretical Study on the Reaction Mechanism via the Minimum Energy Intersystem Crossing Point. Inorganic Chemistry, 2016, 55, 8082-8090.	4.0	8
56	Gold nanoparticles on OMS-2 for heterogeneously catalyzed aerobic oxidative Î±,Î²-dehydrogenation of Î²-heteroatom-substituted ketones. Chemical Communications, 2016, 52, 14314-14317.	4.1	31
57	Highly Active and Robust Metalloporphyrin Catalysts for the Synthesis of Cyclic Carbonates from a Broad Range of Epoxides and Carbon Dioxide. Chemistry - A European Journal, 2016, 22, 6556-6563.	3.3	176
58	A DFT and multi-configurational perturbation theory study on O₂ binding to a model heme compound via the spin-change barrier. Physical Chemistry Chemical Physics, 2016, 18, 18137-18144.	2.8	20
59	Facile Synthesis of 1,4â€Bis(diaryl)â€1,3â€butadiynes Bearing Two Amino Moieties by Electrochemical Reactionâ€Site Switching, and Their Solvatochromic Fluorescence. Asian Journal of Organic Chemistry, 2016, 5, 373-379.	2.7	10
60	Electronic spectra of azaindole and its excited state mixing: A symmetry-adapted cluster configuration interaction study. Journal of Chemical Physics, 2015, 143, 204304.	3.0	5
61	Energy dissipative photoprotective mechanism of carotenoid spheroidene from the photoreaction center of purple bacteria Rhodobacter sphaeroides. Physical Chemistry Chemical Physics, 2015, 17, 23468-23480.	2.8	4
62	Quantum Mechanical Molecular Interactions for Calculating the Excitation Energy in Molecular Environments: A Firstâ€Order Interacting Space Approach. ChemPhysChem, 2015, 16, 305-311.	2.1	9
63	Theoretical Investigation on the Decaying Behavior of Exchange Interaction in Quinoid and Aromatic Molecular Wires. Journal of Physical Chemistry C, 2015, 119, 5117-5121.	3.1	13
64	Quaternary ammonium hydroxide as a metal-free and halogen-free catalyst for the synthesis of cyclic carbonates from epoxides and carbon dioxide. Catalysis Science and Technology, 2015, 5, 2314-2321.	4.1	107
65	mesoâ€Dibenzoporphycene has a Large Bathochromic Shift and a Porphycene Framework with an Unusual cis Tautomeric Form. Angewandte Chemie - International Edition, 2015, 54, 6227-6230.	13.8	46
66	Platinum-catalyzed reduction of amides with hydrosilanes bearing dual Siâ€“H groups: a theoretical study of the reaction mechanism. Dalton Transactions, 2015, 44, 19344-19356.	3.3	22
67	Synergy of Vicinal Oxygenated Groups of Catalysts for Hydrolysis of Cellulosic Molecules. Journal of Physical Chemistry C, 2015, 119, 20993-20999.	3.1	50
68	Computational Investigation into Photoswitching Efficiency of Diarylethene Derivatives: An Insight Based on the Decay Constant of Electron Tunneling. Journal of Physical Chemistry C, 2015, 119, 20169-20178.	3.1	10
69	Entropically Favored Adsorption of Cellulosic Molecules onto Carbon Materials through Hydrophobic Functionalities. ChemSusChem, 2014, 7, 1443-1450.	6.8	91
70	Bifunctional Porphyrin Catalysts for the Synthesis of Cyclic Carbonates from Epoxides and CO₂: Structural Optimization and Mechanistic Study. Journal of the American Chemical Society, 2014, 136, 15270-15279.	13.7	404
71	Investigation on CD Inversion at Visible Region Caused by a Tilt of the Ï€-Conjugated Substituent: Theoretical and Experimental Approaches by Using an Asymmetric Framework of Diarylethene Annulated Isomer. Journal of Physical Chemistry A, 2014, 118, 1084-1093.	2.5	9
72	Excited States of a Significantly Ruffled Porphyrin: Computational Study on Structure-Induced Rapid Decay Mechanism via Intersystem Crossing. Journal of Physical Chemistry A, 2014, 118, 4184-4194.	2.5	18

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73	Theoretical Investigation of the Dependence of Exchange Interaction on Dihedral Angle between Two Aromatic Rings in a Wire Unit. Chemistry Letters, 2014, 43, 530-532.	1.3	9
74	Excitation energy transfer in GFPâ€Xâ€CFP model peptides (X = amino acids): Direct Versus throughâ€bridge energy transfers. International Journal of Quantum Chemistry, 2013, 113, 563-568.	2.0	4
75	Theoretical Investigation of the Î² Value of the Ï€-Conjugated Molecular Wires by Evaluating Exchange Interaction between Organic Radicals. Journal of Physical Chemistry C, 2013, 117, 26280-26286.	3.1	34
76	Fragment-based configuration interaction wave function to calculate environmental effect on excited states in proteins and solutions. Chemical Physics Letters, 2013, 571, 77-81.	2.6	8
77	Theoretical investigation of the Î² value of the phenylene and phenylene ethynylene units by evaluating exchange interaction between organic radicals. Chemical Physics Letters, 2013, 555, 187-190.	2.6	22
78	A Configuration Interaction Picture for a Molecular Environment Using Localized Molecular Orbitals: The Excited States of Retinal Proteins. Journal of Chemical Theory and Computation, 2012, 8, 4452-4461.	5.3	9
79	Sequentially Coupled Holeâ€“Electron Transfer Pathways for Bridge-Mediated Triplet Excitation Energy Transfer. Journal of Physical Chemistry C, 2012, 116, 23252-23256.	3.1	0
80	Kinetic investigation on carbamate formation from the reaction of carbon dioxide with amino acids in homogeneous aqueous solution. Journal of Physical Organic Chemistry, 2012, 25, 239-247.	1.9	20
81	Singlet Excitation Energy Transfer Mediated by Local Exciton Bridges. Journal of Physical Chemistry C, 2012, 116, 13865-13876.	3.1	2
82	Chronological Change from Faceâ€On to Edgeâ€On Ordering of Zincâ€“Tetraphenylporphyrin at the Phenyloctaneâ€“Highly Oriented Pyrolytic Graphite Interface. Chemistry - an Asian Journal, 2012, 7, 394-399.	3.3	9
83	Color Tuning in Human Cone Visual Pigments: The Role of the Protein Environment. Progress in Theoretical Chemistry and Physics, 2012, , 489-502.	0.2	0
84	Bridge-Mediated Excitation Energy Transfer Pathways through Protein Media: a Slater Determinant-Based Electronic Coupling Calculation Combined with Localized Molecular Orbitals. Journal of Physical Chemistry A, 2011, 115, 10814-10822.	2.5	16
85	Theoretical study of the excited states of the photosynthetic reaction center in photosystem II: Electronic structure, interactions, and their origin. Biophysical Chemistry, 2011, 159, 227-236.	2.8	9
86	Theoretical study of the excited states and the redox potentials of unusually distorted Î²-trifluoromethylporphycene. Theoretical Chemistry Accounts, 2011, 130, 175-185.	1.4	4
87	Color Tuning in Photofunctional Proteins. ChemPhysChem, 2011, 12, 3106-3115.	2.1	42
88	Chemical-intuition based LMO transformation simplifies excited-state wave functions of peptides. Chemical Physics Letters, 2011, 508, 171-176.	2.6	12
89	Theoretical Investigation on the Origin of the CD Signal Reversal for the Closed-ring Isomer of Diarylethene with Peripherical Ï€-Conjugated Substituents. Chemistry Letters, 2010, 39, 516-517.	1.3	7
90	Generalizing the bra state in the symmetry-adapted cluster singles and doubles method and the second-order perturbation correction. Chemical Physics Letters, 2010, 486, 84-88.	2.6	1

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91	Excited States of Fluorescent Proteins, mKO and DsRed: Chromophoreâ^'Protein Electrostatic Interaction Behind the Color Variations. Journal of Physical Chemistry B, 2010, 114, 2971-2979.	2.6	43
92	Theoretical study of the opsin shift of deprotonated retinal schiff base in the M state of bacteriorhodopsin. Physical Chemistry Chemical Physics, 2010, 12, 13107.	2.8	16
93	Quantum Chemistry of the Color Tuning Mechanism in the Photobiological System. Molecular Science, 2010, 4, A0031.	0.2	1
94	A multicore QM/MM approach for the geometry optimization of chromophore aggregate in protein. Journal of Computational Chemistry, 2009, 30, 1351-1359.	3.3	10
95	Photocyclization of 2,4,6-triethylbenzophenones in the solid state. Tetrahedron, 2009, 65, 677-689.	1.9	23
96	Artificial color tuning of firefly luminescence: Theoretical mutation by tuning electrostatic interactions between protein and luciferin. Chemical Physics Letters, 2009, 469, 191-194.	2.6	39
97	Charge-Polarized Coordination Space for H₂ Adsorption. Chemistry of Materials, 2009, 21, 1829-1833.	6.7	9
98	A New Synthesis of (+)-Negamycin and Its Derivatives as a Potential Therapeutic Agent for Duchenne Muscular Dystrophy Treatment. Advances in Experimental Medicine and Biology, 2009, 611, 137-138.	1.6	0
99	Circular Dichroism and Absorption Spectroscopy for Three-Membered Ring Compounds Using Symmetry-Adapted Cluster-Configuration Interaction (SAC-CI) Method. Bulletin of the Chemical Society of Japan, 2009, 82, 1215-1226.	3.2	16
100	Color Tuning Mechanism of Human Red, Green, and Blue Cone Pigments: SAC-CI Theoretical Study. Bulletin of the Chemical Society of Japan, 2009, 82, 1140-1148.	3.2	35
101	3P-221 Theoretical Study of Excited States of Photosynthetic Reaction Center in Photosystem II:Structure and Interaction(Photobiology:Photosynthesis,The 47th Annual Meeting of the Biophysical) Tj ETQq1 1 0.784314 rgBT /Ov	0.1	0
102	Origin of color tuning in human red, green, and blue cone pigments: SAC-CI and QM/MM study. Chemical Physics Letters, 2008, 462, 318-320.	2.6	46
103	Exploring Photobiology and Biospectroscopy with the Sac-Ci (Symmetry-Adapted) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 267 Td and Physics, 2008, , 93-124.	0.6	9
104	2P-280 Origin of color tuning in human red, green, and blue cone visual pigments(The 46th Annual) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.1	0
105	Red Light in Chemiluminescence and Yellow-Green Light in Bioluminescence:Â Color-Tuning Mechanism of Firefly,Photinus pyralis, Studied by the Symmetry-Adapted Clusterâ^'Configuration Interaction Method. Journal of the American Chemical Society, 2007, 129, 8756-8765.	13.7	127
106	Theoretical Studies on the Color-Tuning Mechanism in Retinal Proteins. Journal of Chemical Theory and Computation, 2007, 3, 605-618.	5.3	134
107	Excited states of GFP chromophore and active site studied by the SACâ€CI method: Effect of proteinâ€environment and mutations. Journal of Computational Chemistry, 2007, 28, 2443-2452.	3.3	78
108	SAC-CI theoretical study on the excited states of lumiflavin: Structure, excitation spectrum, and solvation effect. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 189, 205-210.	3.9	58

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109	Excited and ionized states of ozone studied by the MEG (multi-exponentially generated)/EX (excited)-MEG method. Chemical Physics, 2007, 332, 262-270.	1.9	12
110	Electronic circular dichroism spectrum of uridine studied by the SACâ€“CI method. Chemical Physics Letters, 2006, 425, 367-371.	2.6	12
111	On the color-tuning mechanism of Human-Blue visual pigment: SAC-CI and QM/MM study. Chemical Physics Letters, 2006, 432, 252-256.	2.6	36
112	On the reversible O2 binding of the Feâ€“porphyrin complex. Journal of Computational Chemistry, 2006, 27, 426-433.	3.3	54
113	On the O2 binding of Feâ€“porphyrin, Feâ€“porphycene, and Feâ€“corrphycene complexes. Journal of Computational Chemistry, 2006, 27, 1363-1372.	3.3	18
114	Photobiology and biospectroscopy studied by SAC-CI method. , 2006, , 1296-1296.		0
115	Excited States and Electron-transfer Mechanism in the Photosynthetic Reaction Center ofRhodobactor sphaeroides: SAC-CI Theoretical Study. Chemistry Letters, 2005, 34, 1242-1243.	1.3	19
116	Generalization of the Projection Space Improves the SAC-SD (symmetry-adapted cluster-singles and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.3	3
117	Mechanism of color tuning in retinal protein: SAC-CI and QM/MM study. Chemical Physics Letters, 2005, 414, 239-242.	2.6	67
118	Structure of phytochromobilin in the Pr and Pfr forms: SAC-CI theoretical study. Chemical Physics Letters, 2005, 410, 90-93.	2.6	15
119	Aza-substitution effect on the Q-band excitations of free-base porphin, chlorin, and bacteriochlorin: SAC-CI theoretical study. Journal of Porphyrins and Phthalocyanines, 2005, 09, 305-315.	0.8	9
120	Excited States of Porphyrin Isomers and Porphycene Derivatives:Â A SAC-CI Study. Journal of Physical Chemistry A, 2005, 109, 3187-3200.	2.5	46
121	Electronic excitations of the green fluorescent protein chromophore in its protonation states: SAC/SAC-CI study. Journal of Computational Chemistry, 2003, 24, 1421-1431.	3.3	83
122	Energetics of the Electron Transfer from Bacteriopheophytin to Ubiquinone in the Photosynthetic Reaction Center of Rhodopseudomonas Viridis:â€‰ Theoretical Study. Journal of Physical Chemistry B, 2003, 107, 838-847.	2.6	19
123	Ground state structure of CuO2: a CASPT2 study. Chemical Physics Letters, 2001, 335, 503-509.	2.6	9
124	Radical cations of perinaphthocyclopropanes. Conditions for the observation of 1,3-perinaphthadiyl radical cationsâ€Šâ€. Perkin Transactions II RSC, 2000, , 2311-2318.	1.1	8
125	Excited States of Free Base Phthalocyanine Studied by the SAC-CI Method. Journal of Physical Chemistry A, 1997, 101, 446-451.	2.5	72
126	SAC-CI study of the excited states of free base tetrazaporphin. Chemical Physics Letters, 1996, 250, 437-442.	2.6	42

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127	Chiral Amino Acid Recognition by a Porphyrin-Based Artificial Receptor. Journal of the American Chemical Society, 1995, 117, 10950-10958.	13.7	108
128	Molecular Trench: Highly Complementary Binding Sites for Tartaric Acid Dialkyl Ester. Journal of the American Chemical Society, 1994, 116, 10338-10339.	13.7	14
129	Revisiting Activity Tuning Using Lattice Strain: CO Decomposition in Terrace Ru(0001) and Stepped Ru(1015) Surfaces. Journal of Physical Chemistry C, 0, , .	3.1	1