Satoshi Maeda

List of Publications by Year
in descending order

210 papers	7,945 citations	53660 45 h-index	64668 79 g-index
231 all docs	231 docs citations	231 times ranked	5222 citing authors

#	Article	IF	Citations
1	Systematic exploration of the mechanism of chemical reactions: the global reaction route mapping (GRRM) strategy using the ADDF and AFIR methods. Physical Chemistry Chemical Physics, 2013, 15, 3683.	1.3	456
2	A scaled hypersphere search method for the topography of reaction pathways on the potential energy surface. Chemical Physics Letters, 2004, 384, 277-282.	1.2	360
3	Global Mapping of Equilibrium and Transition Structures on Potential Energy Surfaces by the Scaled Hypersphere Search Method:â€‰ Applications to ab Initio Surfaces of Formaldehyde and Propyne Molecules. Journal of Physical Chemistry A, 2005, 109, 5742-5753.	1.1	310
4	Intrinsic reaction coordinate: Calculation, bifurcation, and automated search. International Journal of Quantum Chemistry, 2015, 115, 258-269.	1.0	300
5	Global Reaction Route Mapping on Potential Energy Surfaces of Formaldehyde, Formic Acid, and Their Metal-Substituted Analogues. Journal of Physical Chemistry A, 2006, 110, 8933-8941.	1.1	270
6	Development of Azoâ€Based Fluorescent Probes to Detect Different Levels of Hypoxia. Angewandte Chemie - International Edition, 2013, 52, 13028-13032.	7.2	241
7	Finding Reaction Pathways of Type A + B â†’ X: Toward Systematic Prediction of Reaction Mechanisms. Journal of Chemical Theory and Computation, 2011, 7, 2335-2345.	2.3	190
8	Implementation and performance of the artificial force induced reaction method in the GRRM17 program. Journal of Computational Chemistry, 2018, 39, 233-251.	1.5	161
9	Communications: A systematic method for locating transition structures of A+Bâ†’X type reactions. Journal of Chemical Physics, 2010, 132, 241102.	1.2	157
10	Exploring transition state structures for intramolecular pathways by the artificial force induced reaction method. Journal of Computational Chemistry, 2014, 35, 166-173.	1.5	151
11	Updated Branching Plane for Finding Conical Intersections without Coupling Derivative Vectors. Journal of Chemical Theory and Computation, 2010, 6, 1538-1545.	2.3	137
12	Artificial Force Induced Reaction (AFIR) Method for Exploring Quantum Chemical Potential Energy Surfaces. Chemical Record, 2016, 16, 2232-2248.	2.9	125
13	Finding Reaction Pathways for Multicomponent Reactions: The Passerini Reaction is a Fourâ€Component Reaction. Angewandte Chemie - International Edition, 2011, 50, 644-649.	7.2	124
14	Structures of Water Octamers (H2O)8:â€‰ Exploration on Ab Initio Potential Energy Surfaces by the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2007, 111, 4527-4534.	1.1	118
15	No Straight Path: Roaming in Both Ground- and Excited-State Photolytic Channels of NO ₃ â†’ NO + O ₂. Science, 2012, 335, 1075-1078.	6.0	112
16	Computational Catalysis Using the Artificial Force Induced Reaction Method. Accounts of Chemical Research, 2016, 49, 763-773.	7.6	112
17	Automated Global Mapping of Minimal Energy Points on Seams of Crossing by the Anharmonic Downward Distortion Following Method: A Case Study of H₂CO. Journal of Physical Chemistry A, 2009, 113, 1704-1710.	1.1	92
18	From Roaming Atoms to Hopping Surfaces: Mapping Out Global Reaction Routes in Photochemistry. Journal of the American Chemical Society, 2015, 137, 3433-3445.	6.6	91

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19	Mechanochemical synthesis of magnesium-based carbon nucleophiles in air and their use in organic synthesis. Nature Communications, 2021, 12, 6691.	5.8	91
20	Low-Energy Electrocatalytic CO₂ Reduction in Water over Mn-Complex Catalyst Electrode Aided by a Nanocarbon Support and K⁺ Cations. ACS Catalysis, 2018, 8, 4452-4458.	5.5	79
21	Iridium-Catalyzed Asymmetric Borylation of Unactivated Methylene C(sp³)â€“H Bonds. Journal of the American Chemical Society, 2019, 141, 6817-6821.	6.6	79
22	Kinetic prediction of reverse intersystem crossing in organic donorâ€“acceptor molecules. Nature Communications, 2020, 11, 3909.	5.8	75
23	Reaction Mechanism of the Anomalous Formal Nucleophilic Borylation of Organic Halides with Silylborane: Combined Theoretical and Experimental Studies. Journal of the American Chemical Society, 2015, 137, 4090-4099.	6.6	71
24	Electrochemical Dearomative Dicarboxylation of Heterocycles with Highly Negative Reduction Potentials. Journal of the American Chemical Society, 2022, 144, 3685-3695.	6.6	67
25	A new approach for finding a transition state connecting a reactant and a product without initial guess: applications of the scaled hypersphere search method to isomerization reactions of HCN, (H2O)2, and alanine dipeptide. Chemical Physics Letters, 2005, 404, 95-99.	1.2	66
26	Quantum Chemistry Study of H⁺(H₂O)₈:â€‰ A Global Search for Its Isomers by the Scaled Hypersphere Search Method, and Its Thermal Behavior. Journal of Physical Chemistry A, 2007, 111, 10732-10737.	1.1	65
27	Systematic Exploration of Minimum Energy Conical Intersection Structures near the Franckâ€“Condon Region. Journal of Physical Chemistry A, 2014, 118, 12050-12058.	1.1	65
28	Automated exploration of reaction channels. Physica Scripta, 2008, 78, 058122.	1.2	64
29	Water-catalyzed gas-phase reaction of formic acid with hydroxyl radical: A computational investigation. Chemical Physics Letters, 2009, 469, 57-61.	1.2	64
30	Toward Predicting Full Catalytic Cycle Using Automatic Reaction Path Search Method: A Case Study on HCo(CO)3-Catalyzed Hydroformylation. Journal of Chemical Theory and Computation, 2012, 8, 380-385.	2.3	61
31	An Automated and Systematic Transition Structure Explorer in Large Flexible Molecular Systems Based on Combined Global Reaction Route Mapping and Microiteration Methods. Journal of Chemical Theory and Computation, 2009, 5, 2734-2743.	2.3	60
32	Exploring paths of chemical transformations in molecular and periodic systems: An approach utilizing force. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1538.	6.2	59
33	A Theoretical Study on the Photodissociation of Acetone: Insight into the Slow Intersystem Crossing and Exploration of Nonadiabatic Pathways to the Ground State. Journal of Physical Chemistry Letters, 2010, 1, 1841-1845.	2.1	58
34	Silane- and peroxide-free hydrogen atom transfer hydrogenation using ascorbic acid and cobalt-photoredox dual catalysis. Nature Communications, 2021, 12, 966.	5.8	58
35	Global Investigation on the Potential Energy Surface of CH3CN:â€‰ Application of the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2005, 109, 7319-7328.	1.1	57
36	Catalytic Transfer Hydrogenation by a Trivalent Phosphorus Compound: Phosphorusâ€Ligand Cooperation Pathway or P^{III}/P^V Redox Pathway?. Angewandte Chemie - International Edition, 2014, 53, 4633-4637.	7.2	57

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37	Systematic Search for Isomerization Pathways of Hexasilabenzene for Finding Its Kinetic Stability. Organometallics, 2009, 28, 2218-2224.	1.1	56
38	Automated Search for Minimum Energy Conical Intersection Geometries between the Lowest Two Singlet States S₀/S₁-MECIs by the Spin-Flip TDDFT Method. Journal of Chemical Theory and Computation, 2013, 9, 4116-4123.	2.3	56
39	Exploration of minimum energy conical intersection structures of small polycyclic aromatic hydrocarbons: toward an understanding of the size dependence of fluorescence quantum yields. Physical Chemistry Chemical Physics, 2015, 17, 22561-22565.	1.3	56
40	Synthesis and structure of stable base-free dialkylsilanimines. New Journal of Chemistry, 2010, 34, 1637.	1.4	55
41	Exploring the Mechanism of Ultrafast Intersystem Crossing in Rhenium(I) Carbonyl Bipyridine Halide Complexes: Key Vibrational Modes and Spinâ€“Vibronic Quantum Dynamics. Journal of Chemical Theory and Computation, 2016, 12, 2335-2345.	2.3	52
42	No activation barrier synthetic route of glycine from simple molecules (NH3, CH2, and CO2) via carboxylation of ammonium ylide: a theoretical study by the scaled hypersphere search method. Chemical Physics Letters, 2004, 398, 240-244.	1.2	50
43	Insight into Global Reaction Mechanism of [C2, H4, O] System from ab Initio Calculations by the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2007, 111, 5099-5110.	1.1	48
44	Lowest Transition State for the Chirality-Determining Step in Ru((R)-BINAP)-Catalyzed Asymmetric Hydrogenation of Methyl-3-Oxobutanoate. Journal of the American Chemical Society, 2008, 130, 17228-17229.	6.6	48
45	Excited-State Roaming Dynamics in Photolysis of a Nitrate Radical. Journal of Physical Chemistry Letters, 2011, 2, 934-938.	2.1	45
46	Sampling of Transition States for Predicting Diastereoselectivity Using Automated Search Methodâ€”Aqueous Lanthanide-Catalyzed Mukaiyama Aldol Reaction. Journal of Chemical Theory and Computation, 2013, 9, 2882-2886.	2.3	45
47	Deuterium Uptake in Magnetic-Fusion Devices with Lithium-Conditioned Carbon Walls. Physical Review Letters, 2013, 110, 105001.	2.9	45
48	Chiral lanthanide lumino-glass for a circularly polarized light security device. Communications Chemistry, 2020, 3, .	2.0	45
49	Automated exploration of stable isomers of H⁺(H₂O)_n (n = 5â€“7) via ab initio calculations: An application of the anharmonic downward distortion following algorithm. Journal of Computational Chemistry, 2009, 30, 952-961.	1.5	44
50	Anharmonic Downward Distortion Following for Automated Exploration of Quantum Chemical Potential Energy Surfaces. Bulletin of the Chemical Society of Japan, 2014, 87, 1315-1334.	2.0	41
51	Catalytic Hydrogenation of Carbon Dioxide with Ammoniaâ€“Borane by Pincer-Type Phosphorus Compounds: Theoretical Prediction. Journal of the American Chemical Society, 2016, 138, 13481-13484.	6.6	41
52	Reactivity of Gold Clusters in the Regime of Structural Fluxionality. Journal of Physical Chemistry C, 2015, 119, 11120-11130.	1.5	40
53	On Benchmarking of Automated Methods for Performing Exhaustive Reaction Path Search. Journal of Chemical Theory and Computation, 2019, 15, 2111-2115.	2.3	38
54	Photochemical reactions of the low-lying excited states of formaldehyde: T1/S intersystem crossings, characteristics of the S1 and T1 potential energy surfaces, and a global T1 potential energy surface. Journal of Chemical Physics, 2009, 130, 114304.	1.2	37

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55	Exploring Potential Energy Surfaces of Large Systems with Artificial Force Induced Reaction Method in Combination with ONIOM and Microiteration. Journal of Chemical Theory and Computation, 2012, 8, 5058-5063.	2.3	37
56	Kinetic Analysis for the Multistep Profiles of Organic Reactions: Significance of the Conformational Entropy on the Rate Constants of the Claisen Rearrangement. Journal of Physical Chemistry A, 2015, 119, 11641-11649.	1.1	36
57	Generation Mechanisms of Amino Acids in Interstellar Space via Reactions between Closedâ€Shell Species: Significance of Higher Energy Isomers in Molecular Evolution. Astrophysical Journal, 2006, 640, 823-828.	1.6	35
58	Conversion pathways between a fullerene and a ring among C20 clusters by a sphere contracting walk method: Remarkable difference in local potential energy landscapes around the fullerene and the ring. Journal of Chemical Physics, 2006, 124, 174306.	1.2	35
59	Intramolecular vibrational frequencies of water clusters (H2O)nâ€ˆ(n=2â€“5): Anharmonic analyses using potential functions based on the scaled hypersphere search method. Journal of Chemical Physics, 2008, 129, 074315.	1.2	35
60	Introduction of a Luminophore into Generic Polymers via Mechanoradical Coupling with a Prefluorescent Reagent. Angewandte Chemie - International Edition, 2021, 60, 16003-16008.	7.2	35
61	Multistep Intersystem Crossing Pathways in Cinnamate-Based UV-B Sunscreens. Journal of Physical Chemistry Letters, 2016, 7, 4001-4007.	2.1	33
62	Discovery of a synthesis method for a difluoroglycine derivative based on a path generated by quantum chemical calculations. Chemical Science, 2020, 11, 7569-7577.	3.7	33
63	Global analysis of reaction pathways on the potential energy surface of cyanoacetylene by the scaled hypersphere search method. Chemical Physics Letters, 2006, 418, 208-216.	1.2	32
64	Global reaction route mapping on potential energy surfaces of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:m and <mml:math xmlns:mml="http://www.w3.org/1998/Math/. Chemical Physics Letters, 2007, 447, 21-26.	1.2	32
65	A new global reaction route map on the potential energy surface of H2CO with unrestricted level. Chemical Physics Letters, 2008, 460, 55-58.	1.2	32
66	Automated Exploration of Photolytic Channels of HCOOH: Conformational Memory via Excited-State Roaming. Journal of Physical Chemistry Letters, 2012, 3, 1900-1907.	2.1	32
67	Contrasting ring-opening propensities in UV-excited Î±-pyrone and coumarin. Physical Chemistry Chemical Physics, 2016, 18, 2629-2638.	1.3	32
68	Microsolvation of Hydrogen Sulfide:â€‰ Exploration of H₂SÂ·(H₂O)_n and SH⁻Â·H₃O⁺Â·(H₂O)_n₋₁ (n = 5â€“7) Cluster Structures on Ab Initio Potential Energy Surfaces by the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2008, 112, 2962-2968.	1.1	31
69	Finding important anharmonic terms in the sixth-order potential energy function by the scaled hypersphere search method: An application to vibrational analyses of molecules and clusters. Journal of Chemical Physics, 2008, 128, 144111.	1.2	31
70	Theoretical Study on the Photodissociation of Methylamine Involving S₁, T₁, and S₀ States. Journal of Physical Chemistry A, 2013, 117, 5757-5764.	1.1	31
71	A new method for constructing multidimensional potential energy surfaces by a polar coordinate interpolation technique. Chemical Physics Letters, 2003, 381, 177-186.	1.2	30
72	Exploring Multiple Potential Energy Surfaces: Photochemistry of Small Carbonyl Compounds. Advances in Physical Chemistry, 2012, 2012, 1-13.	2.0	29

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73	Azo-Crosslinked Double-Network Hydrogels Enabling Highly Efficient Mechanoradical Generation. Journal of the American Chemical Society, 2022, 144, 3154-3161.	6.6	29
74	Application of Automated Reaction Path Search Methods to a Systematic Search of Single-Bond Activation Pathways Catalyzed by Small Metal Clusters: A Case Study on Hâ€“H Activation by Gold. Journal of Chemical Theory and Computation, 2014, 10, 1623-1630.	2.3	28
75	CASPT2 Study of Photodissociation Pathways of Ketene. Journal of Physical Chemistry A, 2013, 117, 7001-7008.	1.1	27
76	Ab Initio Molecular Dynamics Study of the Photoreaction of 1,1â€²-Dimethylstilbene upon S₀ â†' S₁ Excitation. Journal of Physical Chemistry A, 2016, 120, 8804-8812.	1.1	27
77	Isomerization in Gold Clusters upon O₂ Adsorption. Journal of Physical Chemistry C, 2017, 121, 2661-2668.	1.5	27
78	Rate Constant Matrix Contraction Method for Systematic Analysis of Reaction Path Networks. Chemistry Letters, 2020, 49, 553-564.	0.7	27
79	Understanding CO oxidation on the Pt(111) surface based on a reaction route network. Physical Chemistry Chemical Physics, 2019, 21, 14366-14375.	1.3	27
80	Ab initio Studies on Synthetic Routes of Glycine from Simple Molecules via Ammonolysis of Acetolactone: Applications of the Scaled Hypersphere Search Method. Chemistry Letters, 2004, 33, 1372-1373.	0.7	26
81	Ab initio reaction pathways for photodissociation and isomerization of nitromethane on four singlet potential energy surfaces with three roaming paths. Journal of Chemical Physics, 2014, 140, 244310.	1.2	26
82	Predicting pathways for terpene formation from first principles â€“ routes to known and new sesquiterpenes. Chemical Science, 2014, 5, 1555.	3.7	26
83	Theoretical Study of Hydrogenation Catalysis of Phosphorus Compound and Prediction of Catalyst with High Activity and Wide Application Scope. ACS Catalysis, 2016, 6, 4859-4870.	5.5	26
84	Exploring the full catalytic cycle of rhodium(<scp>i</scp>)â€“BINAP-catalysed isomerisation of allylic amines: a graph theory approach for path optimisation. Chemical Science, 2017, 8, 4475-4488.	3.7	26
85	Analyses of trajectory on-the-fly based on the global reaction route map. Physical Chemistry Chemical Physics, 2018, 20, 1364-1372.	1.3	26
86	A scaled hypersphere interpolation technique for efficient construction of multidimensional potential energy surfaces. Chemical Physics Letters, 2005, 414, 265-270.	1.2	25
87	Automated Exploration of Adsorption Structures of an Organic Molecule on RuH₂â^'BINAP by the ONIOM Method and the Scaled Hypersphere Search Method. Journal of Physical Chemistry A, 2007, 111, 13168-13171.	1.1	25
88	Finding Minimum Structures on the Seam of Crossing in Reactions of Type A + B â†' X: Exploration of Nonadiabatic Ignition Pathways of Unsaturated Hydrocarbons. Journal of Physical Chemistry Letters, 2011, 2, 852-857.	2.1	25
89	Positive Effect of Water in Asymmetric Direct Aldol Reactions with Primary Amine Organocatalyst: Experimental and Computational Studies. Chemistry - an Asian Journal, 2015, 10, 2112-2116.	1.7	24
90	Global search for low-lying crystal structures using the artificial force induced reaction method: A case study on carbon. Physical Review B, 2017, 95, .	1.1	24

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91	One-Minute Joule Annealing Enhances the Thermoelectric Properties of Carbon Nanotube Yarns via the Formation of Graphene at the Interface. ACS Applied Energy Materials, 2019, 2, 7700-7708.	2.5	24
92	A Reaction Path Network for WÃ¶hler's Urea Synthesis. Chemistry Letters, 2019, 48, 47-50.	0.7	24
93	Chemoselective Cleavage of Siâ€“C(sp³) Bonds in Unactivated Tetraalkylsilanes Using Iodine Tris(trifluoroacetate). Journal of the American Chemical Society, 2021, 143, 103-108.	6.6	24
94	Photochemistry of Methyl Ethyl Ketone: Quantum Yields and S₁/S₀â€Diradical Mechanism of Photodissociation. ChemPhysChem, 2010, 11, 3883-3895.	1.0	23
95	Quasiclassical Trajectory Studies of the Photodissociation Dynamics of NO₃ from the D₀ and D₁ Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2013, 9, 893-900.	2.3	23
96	Exploration of Quenching Pathways of Multiluminescent Acenes Using the GRRM Method with the SF-TDDFT Method. Journal of Physical Chemistry A, 2015, 119, 11479-11487.	1.1	23
97	Classical trajectory calculations for collision-energy/electron-energy resolved two-dimensional Penning ionization electron spectra of N2, CO, and CH3CN with metastable He*(2â€Š3S) atoms. Journal of Chemical Physics, 2002, 117, 5707-5721.	1.2	22
98	Long-Range Migration of a Water Molecule To Catalyze a Tautomerization in Photoionization of the Hydrated Formamide Cluster. Journal of Physical Chemistry A, 2010, 114, 11896-11899.	1.1	21
99	Dynamics of deuterium retention and sputtering of Liâ€“Câ€“O surfaces. Fusion Engineering and Design, 2012, 87, 1732-1736.	1.0	20
100	The effect of Mg²⁺ incorporation on the structure of calcium carbonate clusters: investigation by the anharmonic downward distortion following method. Physical Chemistry Chemical Physics, 2016, 18, 2690-2698.	1.3	20
101	Different photoisomerization routes found in the structural isomers of hydroxy methylcinnamate. Physical Chemistry Chemical Physics, 2018, 20, 17583-17598.	1.3	20
102	An overlap expansion method for improvingab initiomodel potentials: Anisotropic intermolecular potentials of N2, CO, and C2H2 with He*(2â€Š3S). Journal of Chemical Physics, 2004, 120, 781-790.	1.2	19
103	Global investigation of potential energy surfaces for the pyrolysis of C₁â€“C₃ hydrocarbons: toward the development of detailed kinetic models from first principles. Physical Chemistry Chemical Physics, 2015, 17, 27789-27805.	1.3	19
104	CO₂ Adsorption on Ti₃O₆^{â€“}: A Novel Carbonate Binding Motif. Journal of Physical Chemistry C, 2019, 123, 8439-8446.	1.5	19
105	Dâ€“L Conversion Pathways between Optical Isomers of Alanine: Applications of the Scaled Hypersphere Search Method to Explore Unknown Reaction Routes in a Chiral System. Chemistry Letters, 2006, 35, 492-493.	0.7	18
106	Global ab Initio Potential Energy Surfaces for Low-Lying Doublet States of NO₃. Journal of Chemical Theory and Computation, 2012, 8, 2600-2605.	2.3	18
107	Combined gradient projection/single component artificial force induced reaction (GP/SC-AFIR) method for an efficient search of minimum energy conical intersection (MECI) geometries. Chemical Physics Letters, 2017, 674, 141-145.	1.2	18
108	Global Reaction Route Mapping for Surface Adsorbed Molecules: A Case Study for H₂O on Cu(111) Surface. Chemistry Letters, 2018, 47, 396-399.	0.7	18

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109	The direct observation of the doorway ¹nÏ€* state of methylcinnamate and hydrogen-bonding effects on the photochemistry of cinnamate-based sunscreens. Physical Chemistry Chemical Physics, 2019, 21, 19755-19763.	1.3	18
110	Combined Automated Reaction Pathway Searches and Sparse Modeling Analysis for Catalytic Properties of Lowest Energy Twins of Cu₁₃. Journal of Physical Chemistry A, 2019, 123, 210-217.	1.1	18
111	Quantum Chemical Calculations to Trace Back Reaction Paths for the Prediction of Reactants. Jacs Au, 2022, 2, 1181-1188.	3.6	18
112	Experimental and theoretical investigations of isomerization reactions of ionized acetone and its dimer. Physical Chemistry Chemical Physics, 2012, 14, 712-719.	1.3	17
113	Analyses of bifurcation of reaction pathways on a global reaction route map: A case study of gold cluster Au5. Journal of Chemical Physics, 2015, 143, 014301.	1.2	17
114	Artificial Force Induced Reaction Method for Systematic Determination of Complex Reaction Mechanisms. Chemical Record, 2016, 16, 2349-2363.	2.9	17
115	Propargylâ€Assisted Selective Amidation Applied in Câ€terminal Glycine Peptide Conjugation. Chemistry - A European Journal, 2016, 22, 18865-18872.	1.7	17
116	Exploring radiative and nonradiative decay paths in indole, isoindole, quinoline, and isoquinoline. Photochemical and Photobiological Sciences, 2018, 17, 315-322.	1.6	17
117	Theoretical study on mechanism of the photochemical ligand substitution of fac-[Re^I(bpy)(CO)₃(PR₃)]⁺ complex. Physical Chemistry Chemical Physics, 2016, 18, 17557-17564.	1.3	16
118	An autocatalytic cycle in autoxidation of triethylborane. Chemical Communications, 2017, 53, 7302-7305.	2.2	16
119	Excess charge driven dissociative hydrogen adsorption on Ti₂O₄^{â˜}. Physical Chemistry Chemical Physics, 2017, 19, 23154-23161.	1.3	16
120	Full rate constant matrix contraction method for obtaining branching ratio of unimolecular decomposition. Journal of Computational Chemistry, 2017, 38, 101-109.	1.5	16
121	Penning ionization electron spectroscopy of C6H6 by collision with He*(2â€Š3S) metastable atoms and classical trajectory calculations: Optimization ofab initiomodel potentials. Journal of Chemical Physics, 2005, 122, 044303.	1.2	15
122	Deciphering Time Scale Hierarchy in Reaction Networks. Journal of Physical Chemistry B, 2016, 120, 1961-1971.	1.2	15
123	Synthesis of Difluoroglycine Derivatives from Amines, Difluorocarbene, and CO₂: Computational Design, Scope, and Applications. Chemistry - A European Journal, 2021, 27, 10040-10047.	1.7	15
124	Collision-energy-resolved Penning ionization electron spectroscopy of OCS with He*(23S) metastable atoms. Chemical Physics Letters, 2003, 379, 332-339.	1.2	14
125	A systematic study on the RuHClâ€“BINAP-catalyzed asymmetric hydrogenation mechanism by the global reaction route mapping methodâ˜†. Journal of Molecular Catalysis A, 2010, 324, 133-140.	4.8	14
126	Observation of Boraneâ€“Olefin Proximity Interaction Governing the Structure and Reactivity of Boronâ€Containing Macrocycles. Angewandte Chemie - International Edition, 2021, 60, 14630-14635.	7.2	14

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127	Ion Chemistry of VX Surrogates and Ion Energetics Properties of VX: New Suggestions for VX Chemical Ionization Mass Spectrometry Detection. Analytical Chemistry, 2010, 82, 3764-3771.	3.2	13
128	Nonadiabatic Pathways of Furan and Dibenzofuran: What Makes Dibenzofuran Fluorescent?. Chemistry Letters, 2016, 45, 940-942.	0.7	13
129	Fluorescence Enhancement of Aromatic Macrocycles by Lowering Excited Singlet State Energies. Journal of Organic Chemistry, 2020, 85, 150-157.	1.7	13
130	Targeted 1,3-dipolar cycloaddition with acrolein for cancer prodrug activation. Chemical Science, 2021, 12, 5438-5449.	3.7	13
131	Substitution effect on the nonradiative decay andtransâ†'cisphotoisomerization route: a guideline to develop efficient cinnamate-based sunscreens. Physical Chemistry Chemical Physics, 2021, 23, 834-845.	1.3	13
132	DFT Study on Isomerization and Decomposition of Cuprous Dialkyldithiophosphate and Its Reaction with Alkylperoxy Radical. Journal of Physical Chemistry A, 2008, 112, 5720-5726.	1.1	12
133	Ab initio anharmonic calculations of vibrational frequencies of benzene by means of efficient construction of potential energy functions. Chemical Physics Letters, 2011, 503, 322-326.	1.2	12
134	Multiple Reaction Pathways Operating in the Mechanism of Vinylogous Mannichâ€Type Reaction Activated by a Water Molecule. Chemistry - an Asian Journal, 2014, 9, 305-312.	1.7	12
135	Palladiumâ€Catalyzed Câ˜H Iodination of Arenes by Means of Sulfinyl Directing Groups. Chemistry - an Asian Journal, 2020, 15, 2442-2446.	1.7	12
136	Classical trajectory calculations of collision energy dependence of Penning ionization cross-sections for N2 and CO by Heâˆ—23S; optimization of anisotropic model potentials. Chemical Physics Letters, 2002, 355, 311-318.	1.2	11
137	Theoretical Investigation of the Reaction Pathway of O Atom on Si(001)-(2 Ã— 1). Journal of Physical Chemistry C, 2010, 114, 15671-15677.	1.5	11
138	Exploration of Isomers of Benzene by GRRM/SCC-DFTB. Chemistry Letters, 2014, 43, 702-704.	0.7	11
139	Zn(OTf)₂-mediated annulations of N-propargylated tetrahydrocarbolines: divergent synthesis of four distinct alkaloidal scaffolds. Chemical Science, 2019, 10, 5686-5698.	3.7	11
140	Exploring approximate geometries of minimum energy conical intersections by TDDFT calculations. Chemical Physics Letters: X, 2019, 737, 100007.	2.1	11
141	Nontotally symmetric trifurcation of an S N 2 reaction pathway. Journal of Computational Chemistry, 2016, 37, 487-493.	1.5	10
142	Ultrafast Nonadiabatic Cascade and Subsequent Photofragmentation of Extreme Ultraviolet Excited Caffeine Molecule. Journal of Physical Chemistry Letters, 2018, 9, 6927-6933.	2.1	10
143	Development of a cooled He*(2S3) beam source for measurements of state-resolved collision energy dependence of Penning ionization cross sections: Evidence for a stereospecific attractive well around methyl group in CH3CN. Journal of Chemical Physics, 2005, 123, 194308.	1.2	9
144	Temperature dependences of rate coefficients for electron catalyzed mutual neutralization. Journal of Chemical Physics, 2011, 135, 024204.	1.2	9

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145	Isomers of Benzene on Its Global Network of Reaction Pathways. Bulletin of the Chemical Society of Japan, 2015, 88, 1284-1290.	2.0	9
146	On-the-fly molecular dynamics study of the excited-state branching reaction of Î±-methyl-cis-stilbene. Chemical Physics, 2018, 515, 564-571.	0.9	9
147	Roles of Closed- and Open-Loop Conformations in Large-Scale Structural Transitions of <scp>l</scp>-Lactate Dehydrogenase. ACS Omega, 2019, 4, 1178-1184.	1.6	9
148	A theoretical study on the alkali metal carboxylateâ€promoted <scp>Lâ€Lactide</scp> polymerization. Journal of Computational Chemistry, 2020, 41, 2197-2202.	1.5	9
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