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	A Dataset of Computational Reaction Barriers for the Claisen Rearrangement: Chemical and Numerical Analysis. Molecular Informatics, 2022, 41, e2100216.	1.4	2
2	Anthraquinodimethane Ring-Flip in Sterically Congested Alkenes: Isolation of Isomer and Elucidation of Intermediate through Experimental and Theoretical Approach. Bulletin of the Chemical Society of Japan, 2022, 95, 38-46.	2.0	5
3	Designing two-dimensional dodecagonal boron nitride. CrystEngComm, 2022, 24, 471-474.	1.3	7
4	Kinetic Analysis of a Reaction Path Network Including Ambimodal Transition States: A Case Study of an Intramolecular Dielsâ€“Alder Reaction. Journal of Chemical Theory and Computation, 2022, 18, 1663-1671.	2.3	2
5	Selecting molecules with diverse structures and properties by maximizing submodular functions of descriptors learned with graph neural networks. Scientific Reports, 2022, 12, 1124.	1.6	4
6	Azo-Crosslinked Double-Network Hydrogels Enabling Highly Efficient Mechanoradical Generation. Journal of the American Chemical Society, 2022, 144, 3154-3161.	6.6	29
7	Leveraging algorithmic search in quantum chemical reaction path finding. Physical Chemistry Chemical Physics, 2022, 24, 10305-10310.	1.3	6
8	Electrochemical Dearomative Dicarboxylation of Heterocycles with Highly Negative Reduction Potentials. Journal of the American Chemical Society, 2022, 144, 3685-3695.	6.6	67
9	Enhancement of the mechanical and thermal transport properties of carbon nanotube yarns by boundary structure modulation. Nanotechnology, 2022, 33, 235707.	1.3	5
10	Virtual Ligand-Assisted Screening Strategy to Discover Enabling Ligands for Transition Metal Catalysis. ACS Catalysis, 2022, 12, 3752-3766.	5.5	8
11	Quantum Chemical Calculations to Trace Back Reaction Paths for the Prediction of Reactants. Jacs Au, 2022, 2, 1181-1188.	3.6	18
12	Designing transformer oil immersion cooling servers for machine learning and first principle calculations. PLoS ONE, 2022, 17, e0266880.	1.1	2
13	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
14	Combined Graph/Relational Database Management System for Calculated Chemical Reaction Pathway Data. Journal of Chemical Information and Modeling, 2021, 61, 554-559.	2.5	6
15	Targeted 1,3-dipolar cycloaddition with acrolein for cancer prodrug activation. Chemical Science, 2021, 12, 5438-5449.	3.7	13
16	Mining hydroformylation in complex reaction networkviagraph theory. RSC Advances, 2021, 11, 23235-23240.	1.7	1
17	Silane- and peroxide-free hydrogen atom transfer hydrogenation using ascorbic acid and cobalt-photoredox dual catalysis. Nature Communications, 2021, 12, 966.	5.8	58
18	Synthesis of a plasmenylethanolamine. Bioscience, Biotechnology and Biochemistry, 2021, 85, 1383-1389.	0.6	3

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19	Nonâ€adiabatic dynamic of atmospheric unimolecular photochemical reactions of 4,4â€difluoroâ€crotonaldehyde using TDâ€DFT and TSH approaches. International Journal of Quantum Chemistry, 2021, 121, e26663.	1.0	2
20	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
21	Observation of Boraneâ€“Olefin Proximity Interaction Governing the Structure and Reactivity of Boronâ€Containing Macrocycles. Angewandte Chemie, 2021, 133, 14751-14756.	1.6	5
22	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
23	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
24	Synthesis of Difluoroglycine Derivatives from Amines, Difluorocarbene, and CO 2 : Computational Design, Scope, and Applications. Chemistry - A European Journal, 2021, 27, 9965-9966.	1.7	0
25	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
26	Pincerâ€Type Phosphorus Compounds With Borylâ€Pendant And Application In Catalytic H 2 Generation From Ammoniaâ€Borane: A Theoretical Study. ChemCatChem, 2021, 13, 3925-3929.	1.8	3
27	Mechanism of 2,6-Dichloro-4,4â€²-bipyridine-Catalyzed Diboration of Pyrazines Involving a Bipyridine-Stabilized Boryl Radical. Bulletin of the Chemical Society of Japan, 2021, 94, 1894-1902.	2.0	3
28	A reaction route network for methanol decomposition on a Pt(111) surface. Journal of Computational Chemistry, 2021, 42, 2163-2169.	1.5	8
29	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
30	Carboxylation of a Palladacycle Formed via C(sp³)â^'H Activation: Theoryâ€Driven Reaction Design. Chemistry - an Asian Journal, 2021, 16, 4072-4080.	1.7	1
31	Radical Difunctionalization of Gaseous Ethylene Guided by Quantum Chemical Calculations: Selective Incorporation of Two Molecules of Ethylene. ACS Omega, 2021, 6, 33846-33854.	1.6	7
32	Mechanochemical synthesis of magnesium-based carbon nucleophiles in air and their use in organic synthesis. Nature Communications, 2021, 12, 6691.	5.8	91
33	Understanding the Acetalization Reaction Based on its Reaction Path Network. ChemSystemsChem, 2020, 2, e1900022.	1.1	2
34	Fluorescence Enhancement of Aromatic Macrocycles by Lowering Excited Singlet State Energies. Journal of Organic Chemistry, 2020, 85, 150-157.	1.7	13
35	Computational searches for crystal structures of dioxides of group 14 elements (CO₂,) Tj ETQq1 1 0.784314 rgBT /Overlo	1.7	4
36	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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37	Kinetic prediction of reverse intersystem crossing in organic donorâ€“acceptor molecules. Nature Communications, 2020, 11, 3909.	5.8	75
38	Chiral lanthanide lumino-glass for a circularly polarized light security device. Communications Chemistry, 2020, 3, .	2.0	45
39	Global Search for Crystal Structures of Carbon under High Pressure. ACS Omega, 2020, 5, 18142-18147.	1.6	7
40	Rate Constant Matrix Contraction Method for Systematic Analysis of Reaction Path Networks. Chemistry Letters, 2020, 49, 553-564.	0.7	27
41	Ineffective OH Pinning of the Flipping Dynamics of a Spherical Guest within a Tightâ€Fitting Tube. Angewandte Chemie - International Edition, 2020, 59, 14570-14576.	7.2	6
42	AFIR explorations of transition states of extended unsaturated systems: automatic location of ambimodal transition states. Physical Chemistry Chemical Physics, 2020, 22, 13942-13950.	1.3	7
43	Palladiumâ€Catalyzed Câ^'H Iodination of Arenes by Means of Sulfinyl Directing Groups. Chemistry - an Asian Journal, 2020, 15, 2442-2446.	1.7	12
44	Migrations and Catalytic Action of Water Molecules in the Ionized Formamideâ€“(H2O)2Cluster. Journal of Physical Chemistry A, 2020, 124, 2802-2807.	1.1	0
45	Ineffective OH Pinning of the Flipping Dynamics of a Spherical Guest within a Tightâ€Fitting Tube. Angewandte Chemie, 2020, 132, 14678-14684.	1.6	4
46	Artificial Force-Induced Reaction Method for Systematic Elucidation of Mechanism and Selectivity in Organometallic Reactions. Topics in Organometallic Chemistry, 2020, , 57-80.	0.7	7
47	Phonon transport probed at carbon nanotube yarn/sheet boundaries by ultrafast structural dynamics. Carbon, 2020, 170, 165-173.	5.4	5
48	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
49	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
50	A Theoretical Study on the Mechanism of the Oxidative Deborylation/Câ€“C Coupling Reaction of Borepin Derivatives. Journal of Organic Chemistry, 2019, 84, 1941-1950.	1.7	8
51	Femtosecond electronic relaxation and real-time vibrational dynamics in 2â€²-hydroxychalcone. Physical Chemistry Chemical Physics, 2019, 21, 5344-5358.	1.3	8
52	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
53	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
54	On Benchmarking of Automated Methods for Performing Exhaustive Reaction Path Search. Journal of Chemical Theory and Computation, 2019, 15, 2111-2115.	2.3	38

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55	Structural and Electronic Properties, Isomerization, and NO Dissociation Reactions on Au, Ag, Cu Clusters. Journal of Computer Chemistry Japan, 2019, 18, 64-69.	0.0	2
56	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
57	A Reaction Path Network for WÃ¶hler's Urea Synthesis. Chemistry Letters, 2019, 48, 47-50.	0.7	24
58	Excitedâ€State Reactivity of [Mn(im)(CO)₃(phen)]⁺: A Structural Exploration. Journal of Computational Chemistry, 2019, 40, 72-81.	1.5	7
59	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
60	A Systematic Study on Bond Activation Energies of NO, N₂, and O₂ on Hexamers of Eight Transition Metals. ChemCatChem, 2019, 11, 1346-1353.	1.8	2
61	Exploring approximate geometries of minimum energy conical intersections by TDDFT calculations. Chemical Physics Letters: X, 2019, 737, 100007.	2.1	11
62	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
63	CO₂ Adsorption on Ti₃O₆^{â€“}: A Novel Carbonate Binding Motif. Journal of Physical Chemistry C, 2019, 123, 8439-8446.	1.5	19
64	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
65	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
66	Designing the Backbone of Hexasilabenzene Derivatives with a High Unimolecular Kinetic Stability. Chemistry - A European Journal, 2018, 24, 12264-12268.	1.7	5
67	Different photoisomerization routes found in the structural isomers of hydroxy methylcinnamate. Physical Chemistry Chemical Physics, 2018, 20, 17583-17598.	1.3	20
68	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
69	Exploring radiative and nonradiative decay paths in indole, isoindole, quinoline, and isoquinoline. Photochemical and Photobiological Sciences, 2018, 17, 315-322.	1.6	17
70	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
71	Theoretical study of initial reactions of amine (CH3) NH(3â^) (nâ€¯=â€¯1, 2, 3) with ozone. Chemical Physics Letters, 2018, 692, 111-116.	1.2	7
72	Analyses of trajectory on-the-fly based on the global reaction route map. Physical Chemistry Chemical Physics, 2018, 20, 1364-1372.	1.3	26

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73	Ultrafast Nonadiabatic Cascade and Subsequent Photofragmentation of Extreme Ultraviolet Excited Caffeine Molecule. Journal of Physical Chemistry Letters, 2018, 9, 6927-6933.	2.1	10
74	Exploring potential crossing seams in periodic systems: Intersystem crossing pathways in the benzene crystal. Journal of Chemical Physics, 2018, 149, 072329.	1.2	4
75	Resolving the excited state relaxation dynamics of guanosine monomers and hydrogen-bonded homodimers in chloroform solution. Chemical Physics, 2018, 515, 480-492.	0.9	2
76	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
77	Isomerization in Gold Clusters upon O₂ Adsorption. Journal of Physical Chemistry C, 2017, 121, 2661-2668.	1.5	27
78	An autocatalytic cycle in autoxidation of triethylborane. Chemical Communications, 2017, 53, 7302-7305.	2.2	16
79	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
80	Transition-Metal-Free Boryl Substitution Using Silylboranes and Alkoxy Bases. Synlett, 2017, 28, 1258-1267.	1.0	3
81	Multistructural microiteration technique for geometry optimization and reaction path calculation in large systems. Journal of Computational Chemistry, 2017, 38, 2213-2221.	1.5	6
82	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
83	Excess charge driven dissociative hydrogen adsorption on Ti₂O₄^â. Physical Chemistry Chemical Physics, 2017, 19, 23154-23161.	1.3	16
84	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
85	Full rate constant matrix contraction method for obtaining branching ratio of unimolecular decomposition. Journal of Computational Chemistry, 2017, 38, 101-109.	1.5	16
86	Lecture Tour upon Receiving the 12th Lectureship Award MBLA. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2017, 75, 367-374.	0.0	0
87	Orbital Energy-Based Reaction Analysis of SN2 Reactions. Computation, 2016, 4, 23.	1.0	5
88	Artificial Force Induced Reaction (AFIR) Method for Exploring Quantum Chemical Potential Energy Surfaces. Chemical Record, 2016, 16, 2232-2248.	2.9	125
89	Nontotally symmetric trifurcation of an S N 2 reaction pathway. Journal of Computational Chemistry, 2016, 37, 487-493.	1.5	10
90	Fragmentation network of doubly charged methionine: Interpretation using graph theory. Journal of Chemical Physics, 2016, 145, 094302.	1.2	3

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91	Computational Catalysis Using the Artificial Force Induced Reaction Method. Accounts of Chemical Research, 2016, 49, 763-773.	7.6	112
92	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
93	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
94	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
95	Artificial Force Induced Reaction Method for Systematic Determination of Complex Reaction Mechanisms. Chemical Record, 2016, 16, 2349-2363.	2.9	17
96	Theoretical insight into the wavelength-dependent photodissociation mechanism of nitric acid. Physical Chemistry Chemical Physics, 2016, 18, 24582-24590.	1.3	4
97	Deciphering Time Scale Hierarchy in Reaction Networks. Journal of Physical Chemistry B, 2016, 120, 1961-1971.	1.2	15
98	Nonadiabatic Pathways of Furan and Dibenzofuran: What Makes Dibenzofuran Fluorescent?. Chemistry Letters, 2016, 45, 940-942.	0.7	13
99	Multistep Intersystem Crossing Pathways in Cinnamate-Based UV-B Sunscreens. Journal of Physical Chemistry Letters, 2016, 7, 4001-4007.	2.1	33
100	Propargylâ€Assisted Selective Amidation Applied in Câ€terminal Glycine Peptide Conjugation. Chemistry - A European Journal, 2016, 22, 18865-18872.	1.7	17
101	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
102	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
103	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
104	Contrasting ring-opening propensities in UV-excited Î±-pyrone and coumarin. Physical Chemistry Chemical Physics, 2016, 18, 2629-2638.	1.3	32
105	Isomers of Benzene on Its Global Network of Reaction Pathways. Bulletin of the Chemical Society of Japan, 2015, 88, 1284-1290.	2.0	9
106	Response to â€œComment on â€˜Analyses of bifurcation of reaction pathways on a global reaction route map: A case study of gold cluster Au5â€â€™ [J. Chem. Phys. 143, 177101 (2015)]. Journal of Chemical Physics, 2015, 143, 177102.	1.2	2
107	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
108	Mechanisms for the Breakdown of Halomethanes through Reactions with Groundâ€State Cyano Radicals. ChemPhysChem, 2015, 16, 181-190.	1.0	6

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109	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
110	Reactivity of Gold Clusters in the Regime of Structural Fluxionality. Journal of Physical Chemistry C, 2015, 119, 11120-11130.	1.5	40
111	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
112	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
113	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
114	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
115	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
116	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
117	Intrinsic reaction coordinate: Calculation, bifurcation, and automated search. International Journal of Quantum Chemistry, 2015, 115, 258-269.	1.0	300
118	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
119	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
120	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
121	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
122	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
123	Complete active space second order perturbation theory (CASPT2) study of N(2D) + H2O reaction paths on D1 and D0 potential energy surfaces: Direct and roaming pathways. Journal of Chemical Physics, 2014, 141, 154303.	1.2	4
124	Predicting pathways for terpene formation from first principles â€“ routes to known and new sesquiterpenes. Chemical Science, 2014, 5, 1555.	3.7	26
125	Theoretical Mechanistic Studies on Methyltrioxorhenium-Catalyzed Olefin Cyclopropanation: Stepwise Transfer of a Terminal Methylene Group. Organometallics, 2014, 33, 3840-3846.	1.1	7
126	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

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127	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
128	Exploration of Isomers of Benzene by GRRM/SCC-DFTB. Chemistry Letters, 2014, 43, 702-704.	0.7	11
129	Direct Pathway for Waterâ€“Gas Shift Reaction in Gas Phase. Chemistry Letters, 2014, 43, 193-195.	0.7	6
130	Automated Search for Chemical Reaction Pathways by the Artificial Force Induced Reaction Method: Toward Practical Applications in Synthetic Organic Chemistry. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2014, 72, 567-579.	0.0	2
131	CASPT2 Study of Photodissociation Pathways of Ketene. Journal of Physical Chemistry A, 2013, 117, 7001-7008.	1.1	27
132	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
133	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
134	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
135	Development of Azoâ€Based Fluorescent Probes to Detect Different Levels of Hypoxia. Angewandte Chemie - International Edition, 2013, 52, 13028-13032.	7.2	241
136	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
137	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
138	Deuterium Uptake in Magnetic-Fusion Devices with Lithium-Conditioned Carbon Walls. Physical Review Letters, 2013, 110, 105001.	2.9	45
139	Exploring Multiple Potential Energy Surfaces: Photochemistry of Small Carbonyl Compounds. Advances in Physical Chemistry, 2012, 2012, 1-13.	2.0	29
140	Experimental and theoretical investigations of isomerization reactions of ionized acetone and its dimer. Physical Chemistry Chemical Physics, 2012, 14, 712-719.	1.3	17
141	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
142	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
143	Dynamics of deuterium retention and sputtering of Liâ€“Câ€“O surfaces. Fusion Engineering and Design, 2012, 87, 1732-1736.	1.0	20
144	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

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145	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
146	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
147	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
148	Excited-State Roaming Dynamics in Photolysis of a Nitrate Radical. Journal of Physical Chemistry Letters, 2011, 2, 934-938.	2.1	45
149	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
150	Automated Exploration of Chemical Reaction Pathways. Molecular Science, 2011, 5, A0042-A0042.	0.2	2
151	Temperature dependences of rate coefficients for electron catalyzed mutual neutralization. Journal of Chemical Physics, 2011, 135, 024204.	1.2	9
152	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
153	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
154	Photochemistry of Methyl Ethyl Ketone: Quantum Yields and S₁/S₀â€Ðiradical Mechanism of Photodissociation. ChemPhysChem, 2010, 11, 3883-3895.	1.0	23
155	Inside Cover: Photochemistry of Methyl Ethyl Ketone: Quantum Yields and S₁/S₀â€Ðiradical Mechanism of Photodissociation (ChemPhysChem 18/2010). ChemPhysChem, 2010, 11, 3774-3774.	1.0	1
156	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
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