Jun Li

List of Publications by Year
in descending order

127	4,233	87723	138251
papers	citations	38 h-index	58 g-index

135	135	135	1805
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Validating experiments for the reaction H₂ + NH₂^{â˜…} by dynamical calculations on an accurate full-dimensional potential energy surface. Physical Chemistry Chemical Physics, 2022, 24, 10160-10167.	1.3	9
2	Nucleophilic Aromatic Substitution of 5-Bromo-1,2,3-triazines with Phenols. Journal of Organic Chemistry, 2022, 87, 2590-2600.	1.7	4
3	Theoretical Investigations for Kinetics of the Chemical Reactions: H + SiCl_x (x = 1, 2, 3). Journal of Physical Chemistry A, 2022, 126, 1689-1700.	1.1	6
4	Permutation-Invariant-Polynomial Neural-Network-Based Î”-Machine Learning Approach: A Case for the HO₂ Self-Reaction and Its Dynamics Study. Journal of Physical Chemistry Letters, 2022, 13, 4729-4738.	2.1	15
5	HClâ€“H₂O dimer: an accurate full-dimensional potential energy surface and fully coupled quantum calculations of intra- and intermolecular vibrational states and frequency shifts. Physical Chemistry Chemical Physics, 2021, 23, 7101-7114.	1.3	28
6	A Full-Dimensional Potential Energy Surface and Dynamics of the Multichannel Reaction between H and HO₂. Journal of Physical Chemistry A, 2021, 125, 1540-1552.	1.1	7
7	Potential energy surfaces for high-energy N + O2 collisions. Journal of Chemical Physics, 2021, 154, 084304.	1.2	23
8	Calculation of Transport Parameters Using ab initio and AMOEBA Polarizable Force Field Methods. Journal of Physical Chemistry A, 2021, 125, 4918-4927.	1.1	2
9	Multistructural Variational Reaction Kinetics of the Simplest Unsaturated Methyl Ester: H-Abstraction from Methyl Acrylate by H, OH, CH₃, and HO₂ Radicals. Journal of Physical Chemistry A, 2021, 125, 5103-5116.	1.1	11
10	Dynamical investigations of the O(³P)â€‰+â€‰H₂O reaction at high collision energies on an accurate full-dimensional potential energy surface. Molecular Physics, 2021, 119, .	0.8	1
11	DClâ€“H₂O, HClâ€“D₂O, and DClâ€“D₂O Dimers: Inter- and Intramolecular Vibrational States and Frequency Shifts from Fully Coupled Quantum Calculations on a Full-Dimensional Neural Network Potential Energy Surface. Journal of Physical Chemistry A, 2021, 125, 6437-6449.	1.1	11
12	Vibrational mode-specificity in the dynamics of the Cl + C2H6 â†’ HCl + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 114303.	1.2	14
13	An accurate full-dimensional potential energy surface for the reaction OH + SO â†’ H + SO₂. Physical Chemistry Chemical Physics, 2021, 23, 487-497.	1.3	12
14	Vibrational energy pooling via collisions between asymmetric stretching excited CO₂: a quasi-classical trajectory study on an accurate full-dimensional potential energy surface. Physical Chemistry Chemical Physics, 2021, 23, 24165-24174.	1.3	2
15	An accurate potential energy surface and ring polymer molecular dynamics study of the Cl + CH₄→ HCl + CH₃reaction. Physical Chemistry Chemical Physics, 2020, 22, 344-353.	1.3	21
16	Kinetic study of the OH + HO₂ → H₂O + O₂ reaction using ring polymer molecular dynamics and quantum dynamics. Physical Chemistry Chemical Physics, 2020, 22, 23657-23664.	1.3	6
17	The Triplet Hydroxyl Radical Complex of Phosphorus Monoxide. Angewandte Chemie - International Edition, 2020, 59, 21949-21953.	7.2	10
18	Energy transfer between vibrationally excited carbon monoxide based on a highly accurate six-dimensional potential energy surface. Journal of Chemical Physics, 2020, 153, 054310.	1.2	24

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19	Ro-vibrational spectra of the simplest deuterated criegee intermediate CD2OO. Chinese Journal of Chemical Physics, 2020, 33, 65-68.	0.6	1
20	Bouncing off walls â€“ widths of exit channels from shallow minima can dominate selectivity control. Chemical Science, 2020, 11, 9937-9944.	3.7	17
21	Advances and New Challenges to Bimolecular Reaction Dynamics Theory. Journal of Physical Chemistry Letters, 2020, 11, 8844-8860.	2.1	46
22	Mode specificity of a multi-channel reaction prototype: Fâ€‰+â€‰CH3OHâ€‰â†’â€‰HFâ€‰+â€‰CH3O/CH2OH. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	14
23	Quantitative Dynamics of the N₂O + C₂H₂ â†’ Oxadiazole Reaction: A Model for 1,3-Dipolar Cycloadditions. ACS Omega, 2020, 5, 23343-23350.	1.6	11
24	Accurate Global Potential Energy Surfaces for the H + CH₃OH Reaction by Neural Network Fitting with Permutation Invariance. Journal of Physical Chemistry A, 2020, 124, 5737-5745.	1.1	40
25	High-Fidelity Potential Energy Surfaces for Gas-Phase and Gasâ€“Surface Scattering Processes from Machine Learning. Journal of Physical Chemistry Letters, 2020, 11, 5120-5131.	2.1	127
26	Many-Body Permutationally Invariant Polynomial Neural Network Potential Energy Surface for N₄. Journal of Chemical Theory and Computation, 2020, 16, 4822-4832.	2.3	40
27	Reaction pathways and kinetics study on a syngas combustion system: CO + HO2in an H2O environment. Physical Chemistry Chemical Physics, 2020, 22, 5797-5806.	1.3	2
28	Exceptional levofloxacin removal using biochar-derived porous carbon sheets: Mechanisms and density-functional-theory calculation. Chemical Engineering Journal, 2020, 387, 124103.	6.6	63
29	Capture of the Sulfur Monoxideâ€“Hydroxyl Radical Complex. Journal of the American Chemical Society, 2020, 142, 2175-2179.	6.6	23
30	Mode Specificity in the OH + HO₂ â†’ H₂O + O₂ Reaction: Enhancement of Reactivity by Exciting a Spectator Mode. Journal of the American Chemical Society, 2020, 142, 3331-3335.	6.6	33
31	Comprehensive Investigations of the Clâ€‰+â€‰CH ₃ OHâ€‰â†’â€‰HClâ€‰+â€‰CH ₃ O/CH ₂ OH Reaction: Validation of Experiment and Dynamic Insights. CCS Chemistry, 2020, 2, 882-894.	4.6	36
32	Theoretical Study for the Ground Electronic State of the Reaction OH + SO â†’ H + SO2. Journal of Physical Chemistry A, 2019, 123, 7218-7227.	1.1	11
33	Stereodynamical control of product branching in multi-channel barrierless hydrogen abstraction of CH₃OH by F. Chemical Science, 2019, 10, 7994-8001.	3.7	24
34	Ring-polymer molecular dynamics studies of thermal rate coefficients for reaction F + H2O â†’ HF + OH. Chinese Journal of Chemical Physics, 2019, 32, 313-318.	0.6	6
35	Rate coefficients and branching ratio for multi-channel hydrogen abstractions from CH3OH by F. Chinese Journal of Chemical Physics, 2019, 32, 84-88.	0.6	12
36	Numerical Simulation of Gas-Liquid Dispersion in A Stirred Tank Agitated by Punched Rigid-Flexible Impeller. International Journal of Chemical Reactor Engineering, 2019, 17, .	0.6	3

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37	A critical comparison of neural network potentials for molecular reaction dynamics with exact permutation symmetry. Physical Chemistry Chemical Physics, 2019, 21, 9672-9682.	1.3	39
38	Photoelectronâ€“Photofragment Coincidence Studies on the Dissociation Dynamics of the OHâ€“CH₄ Complex. Journal of Physical Chemistry A, 2019, 123, 4825-4833.	1.1	8
39	Analysis of heat integration, intermediate reboiler and vapor recompression for the extractive distillation of ternary mixture with two binary azeotropes. Chemical Engineering and Processing: Process Intensification, 2019, 142, 107546.	1.8	31
40	Anomalous kinetics of the reaction between OH and HO₂on an accurate triplet state potential energy surface. Physical Chemistry Chemical Physics, 2019, 21, 12667-12675.	1.3	30
41	Quantum dynamical investigation of product state distributions of the F + CH3OH â†' HF + CH3O reaction via photodetachment of the Fâ¯(HOCH3) anion. Journal of Chemical Physics, 2019, 150, 044301.	1.2	5
42	An accurate full-dimensional permutationally invariant potential energy surface for the interaction between H2O and CO. Physical Chemistry Chemical Physics, 2019, 21, 24101-24111.	1.3	14
43	Combined Experimentalâ€“Theoretical Study of the OH + CO â†' H + CO₂ Reaction Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 1229-1236.	2.1	18
44	Thermal Rate Coefficients and Kinetic Isotope Effects for the Reaction OH + CH₄ â†' H₂O + CH₃ on an ab Initio-Based Potential Energy Surface. Journal of Physical Chemistry A, 2018, 122, 2645-2652.	1.1	16
45	Tracking the energy flow in the hydrogen exchange reaction OH + H₂O â†' H₂O + OH. Physical Chemistry Chemical Physics, 2018, 20, 12543-12556.	1.3	19
46	CFD Simulation of Solid Suspension in a Stirred Reactor Driven by a Dual Punched Rigid-Flexible Impeller. International Journal of Chemical Reactor Engineering, 2018, 16, .	0.6	3
47	Classical Trajectory Study of Collision Energy Transfer between Ne and C₂H₂ on a Full Dimensional Accurate Potential Energy Surface. Journal of Physical Chemistry A, 2018, 122, 1521-1530.	1.1	13
48	Kinetics studies of the Fâ€¯+â€¯HCl â†' HFâ€¯+â€¯Cl reaction on an accurate potential energy surface. Chemical Physics Letters, 2018, 694, 93-101.	1.2	3
49	Improved design and optimization for separating tetrahydrofuranâ€“water azeotrope through extractive distillation with and without heat integration by varying pressure. Chemical Engineering Research and Design, 2018, 133, 303-313.	2.7	50
50	Quasi-classical dynamics investigations of the Fâ€¯+â€¯D 2 Oâ€¯â†'â€¯DFâ€¯+â€¯OD reaction on a full dimensional accurate potential energy surface. Computational and Theoretical Chemistry, 2018, 1130, 1-5.	1.1	2
51	Energy-Saving Reduced-Pressure Extractive Distillation with Heat Integration for Separating the Biazeotropic Ternary Mixture Tetrahydrofuranâ€“Methanolâ€“Water. Industrial & Engineering Chemistry Research, 2018, 57, 13498-13510.	1.8	52
52	Design of Impeller Blades for Intensification of Gas-Liquid Dispersion Process in a Stirred Tank. International Journal of Chemical Reactor Engineering, 2018, 16, .	0.6	0
53	Rotational excitation of the interstellar NH2 radical by H2. Journal of Chemical Physics, 2017, 146, 064309.	1.2	12
54	Solid-liquid mixing performance in a stirred tank with a double punched rigid-flexible impeller coupled with a chaotic motor. Chemical Engineering and Processing: Process Intensification, 2017, 118, 37-46.	1.8	21

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55	Quasi-classical trajectory studies on the full-dimensional accurate potential energy surface for the OH + H2O = H2O + OH reaction. Physical Chemistry Chemical Physics, 2017, 19, 17718-17725.	1.3	30
56	Quantum and quasiclassical dynamics of the multi-channel H + H2S reaction. Journal of Chemical Physics, 2017, 146, 124303.	1.2	18
57	Effects of vibrational excitation on the F + H₂O â†' HF + OH reaction: dissociative photodetachment of overtone-excited [Fâ€"Hâ€"OH]^{â^'}. Chemical Science, 2017, 8, 7821-7833.	3.7	16
58	Numerical simulation of solid-liquid suspension in a stirred tank with a dual punched rigid-flexible impeller. Advanced Powder Technology, 2017, 28, 2723-2734.	2.0	44
59	Intensification of chaotic mixing in a stirred tank with a punched rigid-flexible impeller and a chaotic motor. Chemical Engineering and Processing: Process Intensification, 2017, 122, 1-9.	1.8	19
60	Design of impeller blades for efficient homogeneity of solid-liquid suspension in a stirred tank reactor. Advanced Powder Technology, 2017, 28, 2514-2523.	2.0	35
61	Kinetics and dynamics of the C(³P) + H₂O reaction on a full-dimensional accurate triplet state potential energy surface. Physical Chemistry Chemical Physics, 2017, 19, 23280-23288.	1.3	13
62	Feshbach resonances in the exit channel of the Fâ€‰+â€‰CH3OHâ€‰â†'â€‰HFâ€‰+â€‰CH3O reaction observed using transition-state spectroscopy. Nature Chemistry, 2017, 9, 950-955.	6.6	70
63	Imaging a multidimensional multichannel potential energy surface: Photodetachment of Hâ^'(NH3) and NH4â^'. Journal of Chemical Physics, 2016, 144, 244311.	1.2	19
64	Full-dimensional global potential energy surfaces describing abstraction and exchange for the H + H2S reaction. Journal of Chemical Physics, 2016, 145, 014303.	1.2	28
65	Permutation invariant potential energy surfaces for polyatomic reactions using atomistic neural networks. Journal of Chemical Physics, 2016, 144, 224103.	1.2	48
66	Full-Dimensional Potential Energy Surface and Ro-vibrational Levels of Dioxirane. Journal of Physical Chemistry A, 2016, 120, 2991-2998.	1.1	15
67	Mode specific dynamics in the H2 + SH â†' H + H2S reaction. Physical Chemistry Chemical Physics, 2016, 18, 29113-29121.	1.3	21
68	Potential energy surfaces from high fidelity fitting ofab initiopoints: the permutation invariant polynomial - neural network approach. International Reviews in Physical Chemistry, 2016, 35, 479-506.	0.9	316
69	An accurate multi-channel multi-reference full-dimensional global potential energy surface for the lowest triplet state of H2O2. Physical Chemistry Chemical Physics, 2016, 18, 29825-29835.	1.3	14
70	Ring-polymer molecular dynamical calculations for the F + HCl â†' HF + Cl reaction on the ground 1²Aâ€² potential energy surface. Physical Chemistry Chemical Physics, 2016, 18, 32031-32041.	1.3	14
71	Mode specificity in the OH + CHD3 reaction: Reduced-dimensional quantum and quasi-classical studies on an ab initio based full-dimensional potential energy surface. Journal of Chemical Physics, 2016, 144, 164303.	1.2	15
72	Rate Coefficient for the ⁴HeÎ¼ + CH₄ Reaction at 500 K: Comparison between Theory and Experiment. Journal of Physical Chemistry B, 2016, 120, 1641-1648.	1.2	28

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73	Communication: An accurate full 15 dimensional permutationally invariant potential energy surface for the OH + CH4 â†' H2O + CH3 reaction. Journal of Chemical Physics, 2015, 143, 221103.	1.2	56
74	Mode specific dynamics of the H2 + CH3 â†' H + CH4 reaction studied using quasi-classical trajectory and eight-dimensional quantum dynamics methods. Journal of Chemical Physics, 2015, 143, 154307.	1.2	12
75	Vibrational energy levels of the simplest Criegee intermediate (CH2OO) from full-dimensional Lanczos, MCTDH, and MULTIMODE calculations. Journal of Chemical Physics, 2015, 143, 084311.	1.2	9
76	Permutationally invariant fitting of intermolecular potential energy surfaces: A case study of the Ne-C2H2 system. Journal of Chemical Physics, 2015, 143, 214304.	1.2	23
77	State-Resolved Quantum Dynamics of Photodetachment of HCO₂^{â^'}/DCO₂^{â^'} on an Accurate Global Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 7316-7324.	1.1	8
78	An experimental and theoretical study on rotational constants of vibrationally excited CH2OO. Chemical Physics Letters, 2015, 621, 129-133.	1.2	25
79	Explicitly correlated MRCI-F12 potential energy surfaces for methane fit with several permutation invariant schemes and full-dimensional vibrational calculations. Molecular Physics, 2015, 113, 1823-1833.	0.8	63
80	Near Spectroscopically Accurate Ab Initio Potential Energy Surface for NH₄⁺ and Variational Calculations of Low-Lying Vibrational Levels. Journal of Physical Chemistry A, 2015, 119, 3400-3406.	1.1	10
81	From ab Initio Potential Energy Surfaces to State-Resolved Reactivities: X + H2O â†" HX + OH [X = F, Cl, and O(3P)] Reactions. Journal of Physical Chemistry A, 2015, 119, 4667-4687.	1.1	90
82	A permutationally invariant full-dimensional ab initio potential energy surface for the abstraction and exchange channels of the H + CH4 system. Journal of Chemical Physics, 2015, 142, 204302.	1.2	71
83	Final state-resolved mode specificity in HX + OH â†' X + H₂O (X = F and Cl) reactions: A quasi-classical trajectory study. Journal of Chemical Physics, 2015, 142, 084314.	1.2	27
84	Infrared spectrum of the simplest Criegee intermediate CH2OO at resolution 0.25 cmâ^'1 and new assignments of bands 2Î½9 and Î½5. Journal of Chemical Physics, 2015, 142, 214301.	1.2	37
85	Insights into the bond-selective reaction of Cl + HOD(n_{OH}) â†' HCl + OD. Physical Chemistry Chemical Physics, 2015, 17, 4259-4267.	1.3	32
86	Quantum and quasi-classical dynamics of the OH + CO â†' H + CO2 reaction on a new permutationally invariant neural network potential energy surface. Journal of Chemical Physics, 2014, 140, 044327.	1.2	60
87	Imaging Dynamics on the F + H ₂ O â†' HF + OH Potential Energy Surfaces from Wells to Barriers. Science, 2014, 343, 396-399.	6.0	93
88	Full-dimensional characterization of photoelectron spectra of HOCOâ^' and DOCOâ^' and tunneling facilitated decay of HOCO prepared by anion photodetachment. Journal of Chemical Physics, 2014, 140, 184314.	1.2	20
89	Hemibond complexes between H2S and free radicals (F, Cl, Br, and OH). Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	9
90	Mode specificity in the HF + OH â†' F + H2O reaction. Journal of Chemical Physics, 2014, 141, 164316.	1.2	19

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91	Nine-dimensional quantum dynamics study of the H₂+ NH₂â†' H + NH₃reaction: a rigorous test of the sudden vector projection model. Physical Chemistry Chemical Physics, 2014, 16, 17770.	1.3	22
92	A nine-dimensional global potential energy surface for NH₄(X²A₁) and kinetics studies on the H + NH₃â†" H₂+ NH₂reaction. Physical Chemistry Chemical Physics, 2014, 16, 6753-6763.	1.3	52
93	Effects of reactant rotation on the dynamics of the OH + CH4 â†' H2O + CH3 reaction: A six-dimensional study. Journal of Chemical Physics, 2014, 140, 084307.	1.2	40
94	Effects of reactant rotational excitation on reactivity: Perspectives from the sudden limit. Journal of Chemical Physics, 2014, 140, 034112.	1.2	49
95	High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH₂OO). Journal of Physical Chemistry Letters, 2014, 5, 2364-2369.	2.1	86
96	A comparison study of the HÂ+ÂCH4 and HÂ+ÂSiH4 reactions with eight-dimensional quantum dynamics: normal mode versus local mode in the reactant molecule vibration. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6
97	Mode Specificity and Product Energy Disposal in Unimolecular Reactions: Insights from the Sudden Vector Projection Model. Journal of Physical Chemistry A, 2014, 118, 2419-2425.	1.1	29
98	Tunneling in Unimolecular and Bimolecular Reactions. Physical Chemistry in Action, 2014, , 59-80.	0.1	0
99	Mode selectivity in methane dissociative chemisorption on Ni(111). Chemical Science, 2013, 4, 3249.	3.7	115
100	Iron cation catalyzed reduction of N2O by CO: gas-phase temperature dependent kinetics. Physical Chemistry Chemical Physics, 2013, 15, 11257.	1.3	26
101	Spin-orbit corrected full-dimensional potential energy surfaces for the two lowest-lying electronic states of FH2O and dynamics for the F + H2O â†' HF + OH reaction. Journal of Chemical Physics, 2013, 138, 074309.	1.2	43
102	Quantum Manifestation of Roaming in H + MgH â†' Mg + H₂: The Birth of Roaming Resonances. Journal of Physical Chemistry A, 2013, 117, 5052-5060.	1.1	41
103	CO₂ Vibrational State Distributions From Quasi-Classical Trajectory Studies of the HO + CO â†' H + CO₂ Reaction and H + CO₂ Inelastic Collision. Journal of Physical Chemistry A, 2013, 117, 11648-11654.	1.1	16
104	Reactant Vibrational Excitations Are More Effective than Translational Energy in Promoting an Early-Barrier Reaction FÂ+ÂH₂O â†' HFÂ+ÂOH. Journal of the American Chemical Society, 2013, 135, 982-985.	6.6	77
105	Enhancement of bimolecular reactivity by a pre-reaction van der Waals complex: the case of F + H2O â†' HF + HO. Chemical Science, 2013, 4, 629-632.	3.7	57
106	Accurate Determination of Barrier Height and Kinetics for the F + H₂O â†' HF + OH Reaction. Journal of Physical Chemistry A, 2013, 117, 8864-8872.	1.1	53
107	Kinetic and dynamic studies of the Cl(2Pu) + H2O($ilde X$XÌƒ1A1) â†' HCl($ilde X$XÌƒ1Î£+) + OH($ilde X$XÌƒ2Î) reaction on an ab initio based full-dimensional global potential energy surface of the ground electronic state of ClH2O. Journal of Chemical Physics, 2013, 139, 074302.	1.2	42
108	Quasi-classical Trajectory Study of F+H2Oâ†'HF+OH Reaction: Influence of Barrier Height, Reactant Rotational Excitation, and Isotopic Substitution. Chinese Journal of Chemical Physics, 2013, 26, 627-634.	0.6	29

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109	Effects of reactant internal excitation and orientation on dissociative chemisorption of H2O on Cu(111): Quasi-seven-dimensional quantum dynamics on a refined potential energy surface. Journal of Chemical Physics, 2013, 138, 044704.	1.2	57
110	Communication: Covalent nature of Xâ‹¯H2O (X = F, Cl, and Br) interactions. Journal of Chemical Physics, 2013, 138, 141102.	1.2	50
111	Rate coefficients and kinetic isotope effects of the X + CH4 â† ' CH3 + HX (X = H, D, Mu) reactions from ring polymer molecular dynamics. Journal of Chemical Physics, 2013, 138, 094307.	1.2	72
112	A new ab initio based global HOOH(13Aâ€³) potential energy surface for the O(3P) + H2O(X1A1) â† " OH(X2Î) + OH(X2Î) reaction. Journal of Chemical Physics, 2013, 138, 194304.	1.2	24
113	Permutation invariant polynomial neural network approach to fitting potential energy surfaces. II. Four-atom systems. Journal of Chemical Physics, 2013, 139, 204103.	1.2	269
114	Quasi-classical trajectory study of the H + CO2 â† ' HO + CO reaction on a new ab initio based potential energy surface. Journal of Chemical Physics, 2012, 137, 024308.	1.2	23
115	Tunneling Facilitated Dissociation fo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold">H</mml:mi><mml:mo mathvariant="bold">+</mml:mo><mml:msub><mml:mi>CO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>HOCO</mml:mi><mml:mo>â^'</mml:mo></mml:msup></mml:math>Photodetachment. Physical Review Letters, 2012, 109, 063202.	2.9	28
116	An ab initio based full-dimensional global potential energy surface for FH2O(X2Aâ€²) and dynamics for the F + H2O â† ' HF + HO reaction. Journal of Chemical Physics, 2012, 137, 094304.	1.2	70
117	Mode Selectivity for a â€œCentralâ€•Barrier Reaction: Eight-Dimensional Quantum Studies of the O(³P) + CH₄ â† ' OH + CH₃ Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry Letters, 2012, 3, 3776-3780.	2.1	87
118	Kinetic study of the formation of triphenylene from the condensation of C12H10+C6H5. Computational and Theoretical Chemistry, 2012, 985, 1-7.	1.1	13
119	Communication: A chemically accurate global potential energy surface for the HO + CO â† ' H + CO2 reaction. Journal of Chemical Physics, 2012, 136, 041103.	1.2	102
120	Quantum Dynamics of the HO + CO â† ' H + CO2 Reaction on an Accurate Potential Energy Surface. Journal of Physical Chemistry Letters, 2012, 3, 2482-2486.	2.1	40
121	Quasi-Classical Trajectory Study of the HO + CO â† ' H + CO₂ Reaction on a New ab Initio Based Potential Energy Surface. Journal of Physical Chemistry A, 2012, 116, 5057-5067.	1.1	51
122	Investigations on the Kinetics for the Reaction Class of Hydrogen Abstractions from Substituted Cyclohexane by Hydrogen Atom. Acta Chimica Sinica, 2012, 70, 585.	0.5	0
123	A theoretical search for stable bent and linear structures of low-lying electronic states of the titanium dioxide (TiO2) molecule. RSC Advances, 2011, 1, 1228.	1.7	10
124	Computational Study of the Reaction Mechanism of the Methylperoxy Self-Reaction. Journal of Physical Chemistry A, 2011, 115, 13534-13541.	1.1	33
125	Unimolecular decomposition mechanism of vinyl alcohol by computational study. Theoretical Chemistry Accounts, 2011, 128, 341-348.	0.5	11
126	Symmetry forbidden vibronic spectra and internal conversion in benzene. Physical Chemistry Chemical Physics, 2010, 12, 14967.	1.3	31

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127	Solvent reorganization energy of electron transfer by a modified ellipsoidal cavity model. Computational and Theoretical Chemistry, 2007, 819, 32-40.	1.5	0