Minghui Yang

List of Publications by Year
in descending order

79 papers	2,303 citations	218677 26 h-index	233421 45 g-index
79 all docs	79 docs citations	79 times ranked	1489 citing authors

#	Article	IF	Citations
1	Toward a Comprehensive Understanding of Mode-Specific Dynamics of Polyatomic Reactions: A Full-Dimensional Quantum Dynamics Study of the H + NH3 Reaction. Journal of Physical Chemistry A, 2022, 126, 663-669.	2.5	6
2	Ten-dimensional quantum dynamics study of H+CH₃D â†' H₂+CH₂D reaction. Chinese Journal of Chemical Physics, 2022, 35, 213-218.	1.3	1
3	Mode-specific quantum dynamics study of OH + H₂S â†' H₂O + SH reaction. Chinese Journal of Chemical Physics, 2022, 35, 200-206.	1.3	5
4	A novel hybrid machine learning model for predicting rate constants of the reactions between alkane and CH3 radical. Fuel, 2022, 322, 124150.	6.4	7
5	Ultrafast Proton Transfer of the Aqueous Phenol Radical Cation. Physical Chemistry Chemical Physics, 2022, , .	2.8	1
6	Coloring ultrasensitive MRI with tunable metalâ€“organic frameworks. Chemical Science, 2021, 12, 4300-4308.	7.4	15
7	Predicting Rate Constants of Hydroxyl Radical Reactions with Alkanes Using Machine Learning. Journal of Chemical Information and Modeling, 2021, 61, 4259-4265.	5.4	20
8	Effects of bending excitation on the reaction dynamics of fluorine atoms with ammonia. Physical Chemistry Chemical Physics, 2021, 23, 2715-2722.	2.8	7
9	Dissociative photodetachment of H₃O₂^{â^'}: a full-dimensional quantum dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 22298-22304.	2.8	2
10	The regulation mechanism of phosphorylation and mutations in intrinsically disordered protein 4E-BP2. Physical Chemistry Chemical Physics, 2020, 22, 2938-2948.	2.8	5
11	Final-State-Resolved Dynamics of the H₃⁺ + CO â†' H₂+HCO⁺/HOC⁺ Reaction: A Quasi-Classical Trajectory Study. Journal of Physical Chemistry A, 2020, 124, 6794-6800.	2.5	5
12	Mode- and Bond-Selected Reaction of H with Local Mode Molecule HDS. Journal of Physical Chemistry A, 2020, 124, 10162-10170.	2.5	4
13	<scp>C1188D</scp> mutation abolishes specific recognition between <scp>MLL1â€CXXC</scp> domain and <scp>CpG</scp> site by inducing conformational switch of flexible Nâ€terminal. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1401-1412.	2.6	1
14	An Ultraviolet Thermally Activated Delayed Fluorescence OLED with Total External Quantum Efficiency over 9%. Advanced Materials, 2020, 32, e2001248.	21.0	134
15	A ten-dimensional quantum dynamics model for the X + YCAB2 reaction: Application to H + CH4 reaction. Journal of Chemical Physics, 2020, 153, 224119.	3.0	6
16	Theoretical studies of strong-field photoionization of CH3I. Chemical Physics, 2019, 516, 28-32.	1.9	0
17	Investigating the influence of intramolecular bond lengths on the intermolecular interaction of H2â€“AgCl complex: Binding energy, intermolecular vibrations, and isotope effects. Journal of Chemical Physics, 2019, 150, 164301.	3.0	2
18	Kinetic and dynamic studies of the H3+ + CO â†' H2 + HCO+/HOC+ reaction on a high-level ab initio potential energy surface. Journal of Chemical Physics, 2019, 151, .	3.0	12

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19	The Observation of Ligand-Binding-Relevant Open States of Fatty Acid Binding Protein by Molecular Dynamics Simulations and a Markov State Model. International Journal of Molecular Sciences, 2019, 20, 3476.	4.1	18
20	Structure-guided post-SELEX optimization of an ochratoxin A aptamer. Nucleic Acids Research, 2019, 47, 5963-5972.	14.5	51
21	Theoretical study of the F(²P) + NH₃â†' HF + NH₂reaction on an accurate potential energy surface: dynamics and kinetics. Physical Chemistry Chemical Physics, 2019, 21, 11385-11394.	2.8	21
22	Freeâ€base porphyrins as CEST MRI contrast agents with highly upfield shifted labile protons. Magnetic Resonance in Medicine, 2019, 82, 577-585.	3.0	14
23	Ultrafast dissociative ionization and large-amplitude vibrational wave packet dynamics of strong-field-ionized di-iodomethane. Journal of Chemical Physics, 2019, 151, 214308.	3.0	7
24	Understanding rotational mode specificity in the O(3P)+CHD3â†' OH+CD3 reaction by simple reactant alignment pictures. Chinese Journal of Chemical Physics, 2019, 32, 46-52.	1.3	5
25	Machine learning of the rate constants for the reaction between alkanes and hydrogen/oxygen atom. Communications in Information and Systems, 2019, 19, 391-403.	0.5	3
26	Tracking the energy flow in the hydrogen exchange reaction OH + H₂O â†' H₂O + OH. Physical Chemistry Chemical Physics, 2018, 20, 12543-12556.	2.8	19
27	Tracking Ultrafast Bond Dissociation Dynamics at 0.1 Ã... Resolution by Femtosecond Extreme Ultraviolet Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 5742-5747.	4.6	9
28	Dynamics and kinetics of the reaction OH + H₂S â†' H₂O + SH on an accurate potential energy surface. Physical Chemistry Chemical Physics, 2018, 20, 26315-26324.	2.8	25
29	Understanding mode-specific dynamics in the local mode representation. Physical Chemistry Chemical Physics, 2018, 20, 19647-19655.	2.8	10
30	New Method To Extract Final-State Information of Polyatomic Reactions Based on Normal Mode Analysis. Journal of Physical Chemistry A, 2018, 122, 6997-7005.	2.5	17
31	Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). Journal of Chemical Physics, 2018, 149, 044703.	3.0	15
32	A rigorous full-dimensional quantum dynamics study of tunneling splitting of rovibrational states of vinyl radical C2H3. Journal of Chemical Physics, 2017, 146, 224307.	3.0	15
33	Competition between the H- and D-atom transfer channels in the H₂O⁺ + HD reaction: reduced-dimensional quantum and quasi-classical studies. Physical Chemistry Chemical Physics, 2017, 19, 17396-17403.	2.8	9
34	Quantum and quasiclassical dynamics of the multi-channel H + H2S reaction. Journal of Chemical Physics, 2017, 146, 124303.	3.0	18
35	Facile Access to Twisted Intramolecular Chargeâ€Transfer Fluorogens Bearing Highly Pretwisted Donorâ€"Acceptor Systems Together with Readily Fineâ€Tuned Chargeâ€Transfer Characters. Small, 2017, 13, 1604113.	10.0	32
36	Elucidating the origins of multimode vibrational coherences of polyatomic molecules induced by intense laser fields. Nature Communications, 2017, 8, 735.	12.8	54

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37	Structural Properties of Human IAPP Dimer in Membrane Environment Studied by All-Atom Molecular Dynamics Simulations. Scientific Reports, 2017, 7, 7915.	3.3	17
38	Breakdown of the vibrationally adiabatic approximation in the early-barrier CH3Â+ÂHBrÂâ†'ÂCH4Â+ÂBr reaction. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
39	Full-dimensional quantum dynamics study of the H2 + C2H â†' H + C2H2 reaction on an ab initio potential energy surface. Journal of Chemical Physics, 2016, 144, 194309.	3.0	19
40	Communication: Mode specific quantum dynamics of the F + CHD3 â†' HF + CD3 reaction. Journal of Chemical Physics, 2016, 144, 171101.	3.0	47
41	Communication: Equivalence between symmetric and antisymmetric stretching modes of NH3 in promoting H + NH3 â†' H2 + NH2 reaction. Journal of Chemical Physics, 2016, 145, 131101.	3.0	25
42	A Network of Conformational Transitions Revealed by Molecular Dynamics Simulations of the Binary Complex of Escherichia coli 6-Hydroxymethyl-7,8-dihydropterin Pyrophosphokinase with MgATP. Biochemistry, 2016, 55, 6931-6939.	2.5	8
43	Quantum dynamics of water dissociative chemisorption on rigid Ni(111): An approximate nine-dimensional treatment. Journal of Chemical Physics, 2016, 144, 164706.	3.0	36
44	Mode specific dynamics in the H2 + SH â†' H + H2S reaction. Physical Chemistry Chemical Physics, 2016, 18, 29113-29121.	2.8	21
45	Mode-Specific S_N2 Reaction Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 3322-3327.	4.6	63
46	Structural Diversity of Ligand-Binding Androgen Receptors Revealed by Microsecond Long Molecular Dynamics Simulations and Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 4611-4619.	5.3	51
47	State-to-State Mode Specificity in F + CHD₃ â†' HF/DF + CD₃/CHD₂ Reaction. Journal of Physical Chemistry A, 2016, 120, 6521-6528.	2.5	18
48	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.	3.0	15
49	Quantum dynamics of polyatomic dissociative chemisorption on transition metal surfaces: mode specificity and bond selectivity. Chemical Society Reviews, 2016, 45, 3621-3640.	38.1	140
50	Theoretical studies for the N2â€"N2O van der Waals complex: The potential energy surface, intermolecular vibrations, and rotational transition frequencies. Journal of Chemical Physics, 2015, 143, 154304.	3.0	11
51	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.	3.0	12
52	An eight-dimensional quantum dynamics study of the Cl + CH4â†' HCl + CH3 reaction. Journal of Chemical Physics, 2015, 143, 134305.	3.0	36
53	Time-Dependent Wave Packet Study of the H₂ + CH₃ â†' H + CH₄ Reaction. Journal of Physical Chemistry A, 2015, 119, 12480-12484.	2.5	9
54	Molecular Dynamics Simulations of the Escherichia coli HPPK Apo-enzyme Reveal a Network of Conformational Transitions. Biochemistry, 2015, 54, 6734-6742.	2.5	12

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55	Rotational mode specificity in the Cl + CHD3 â†' HCl + CD3 reaction. Journal of Chemical Physics, 2014, 141, 074310.	3.0	75
56	Theoretical prediction of the linear isomers for rare gas-carbon disulfide complexes: He-CS2, Ne-CS2, and Ar-CS2. Journal of Chemical Physics, 2014, 140, 114310.	3.0	25
57	A novel fluorescent pH probe with valuable pK_abased on a twisted intramolecular charge transfer mechanism, and its applications in cell imaging. RSC Advances, 2014, 4, 36849-36853.	3.6	25
58	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.	3.0	40
59	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.	1.4	6
60	Ring Polymer Molecular Dynamics Calculations of Thermal Rate Constants for the O(³P) + CH₄ â†' OH + CH₃ Reaction: Contributions of Quantum Effects. Journal of Physical Chemistry Letters, 2013, 4, 48-52.	4.6	68
61	Isotope effects on the dynamics properties and reaction mechanism in the Cl(2P)Â+ÂNH3 reaction: a QCT and QM study. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	6
62	Mode selectivity in methane dissociative chemisorption on Ni(111). Chemical Science, 2013, 4, 3249.	7.4	115
63	Accelerating modified Shepard interpolated potential energy calculations using graphics processing units. Computer Physics Communications, 2013, 184, 1150-1154.	7.5	3
64	Six-dimensional and seven-dimensional quantum dynamics study of the OH + CH4 â†' H2O + CH3 reaction. Journal of Chemical Physics, 2013, 139, 154310.	3.0	20
65	Full-dimensional quantum calculations of the vibrational states of H5+. Journal of Chemical Physics, 2013, 138, 124309.	3.0	20
66	An eight-dimensional quantum mechanical Hamiltonian for X + YCZ3 system and its applications to H + CH4 reaction. Journal of Chemical Physics, 2012, 137, 174113.	3.0	53
67	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.	4.6	87
68	The structural stability of polyhydroxylated C60(OH)24: Density functional theory characterizations. Computational and Theoretical Chemistry, 2011, 974, 16-20.	2.5	35
69	Kinetics and dynamics of the NH3 + H â†' NH2 + H2 reaction using transition state methods, quasi-classical trajectories, and quantum-mechanical scattering. Journal of Chemical Physics, 2011, 135, 014303.	3.0	26
70	Full dimensional time-dependent quantum dynamics study of the H+NH3â†'H2+NH2 reaction. Journal of Chemical Physics, 2008, 129, 064315.	3.0	43
71	Seven-dimensional quantum dynamics study of the O(P3)+CH4 reaction. Journal of Chemical Physics, 2007, 126, 064303.	3.0	78
72	Seven dimensional quantum dynamics study of the H2+NH2â†'H+NH3 reaction. Journal of Chemical Physics, 2007, 127, 184308.	3.0	16

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73	Seven-dimensional quantum dynamics study of the H+NH3â†'H2+NH2 reaction. Journal of Chemical Physics, 2007, 126, 214312.	3.0	30
74	A seven-dimensional quantum study of the H+CH4 reaction. Journal of Chemical Physics, 2002, 117, 9539-9542.	3.0	121
75	Quantum dynamics of the D2+OH reaction. Journal of Chemical Physics, 2002, 116, 2388-2394.	3.0	37
76	Accuracy of the centrifugal sudden approximation in the H+H2O reaction and accurate integral cross sections for the H+H2Oâ†'H2+OH abstraction reaction. Journal of Chemical Physics, 2002, 117, 10067-10072.	3.0	44
77	Branching ratio in the HD+OH reaction: A full-dimensional quantum dynamics study on a new ab initio potential energy surface. Journal of Chemical Physics, 2001, 114, 8733-8736.	3.0	36
78	Ab initio potential-energy surfaces for the reactions OH+H2â†"H2O+H. Journal of Chemical Physics, 2001, 115, 174-178.	3.0	109
79	Quantum dynamics on new potential energy surfaces for the H2+OHâ†'H2O+H reaction. Journal of Chemical Physics, 2001, 114, 4759-4762.	3.0	64