

# Maodu Chen

## List of Publications by Year in descending order

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76  
papers

1,225  
citations

430874

18  
h-index

434195

31  
g-index

77  
all docs

77  
docs citations

77  
times ranked

1198  
citing authors

#	ARTICLE	IF	CITATIONS
1	Non-adiabatic couplings induced complex-forming mechanism in $H+MgH+ \hat{\sigma}^+ Mg++H_2$ reaction. Chinese Journal of Chemical Physics, 2022, 35, 345-352.	1.3	1
2	Representing globally accurate reactive potential energy surfaces with complex topography by combining Gaussian process regression and neural networks. Physical Chemistry Chemical Physics, 2022, 24, 12827-12836.	2.8	4
3	Stereodynamics-Controlled Product Branching in the Nonadiabatic $H + NaD \hat{\sigma}^+ Na(3s, 3p) + HD$ Reaction at Low Temperatures. Journal of Physical Chemistry A, 2022, 126, 2453-2462.	2.5	6
4	Wave Packet Approach to Adiabatic and Nonadiabatic Dynamics of Cold Inelastic Scatterings. Molecules, 2022, 27, 2912.	3.8	4
5	Time-dependent wave packet dynamics study of the resonances in the $H + LiH \langle \sup \rangle \langle \sup \rangle \langle i \rangle \nu \langle i \rangle = 0$ , $T_j$ ETQq1 1 0.784314 rgBT Chemical Physics, 2022, 24, 15532-15539.	2.8	7
6	Dramatically Enhanced Second Harmonic Generation in Janus Group $\hat{\sigma}^+ III$ Chalcogenide Monolayers. Advanced Optical Materials, 2022, 10, .	7.3	8
7	Time-dependent wave packet dynamics study of non-adiabatic $Li(2p)\hat{\sigma}^+ \hat{\sigma}^+ HD\hat{\sigma}^+ \hat{\sigma}^+ LiH/LiD\hat{\sigma}^+ \hat{\sigma}^+ H$ reaction in a diabatic representation. Chemical Physics Letters, 2021, 764, 138279.	2.6	1
8	Transition metal-doped $Bn$ ( $n \hat{\sigma}^+ \% = \hat{\sigma}^+ \% 7 \hat{\sigma}^+ 10$ ) clusters: confirmation of a circular disk Jellium model. European Physical Journal Plus, 2021, 136, 1.	2.6	5
9	Noble Metallic Pyramidal Substrate for Surface-Enhanced Raman Scattering Detection of Plasmid DNA Based on Template Stripping Method. Micromachines, 2021, 12, 923.	2.9	0
10	Inelastic, exchange, and reactive processes in rovibrationally excited collisions of HD with H. Monthly Notices of the Royal Astronomical Society, 2021, 507, 6012-6019.	4.4	4
11	Non-adiabatic quantum dynamics studies of the $Mg+(3p)\hat{\sigma}^+ \hat{\sigma}^+ D_2\hat{\sigma}^+ \hat{\sigma}^+ MgD+\hat{\sigma}^+ \hat{\sigma}^+ D$ reaction. Chemical Physics, 2021, 550, 111311.	1.9	1
12	Evolution of Water Layer Adsorption on the GaN(0001) Surface and Its Influence on Electronic Properties. Journal of Physical Chemistry C, 2021, 125, 667-674.	3.1	5
13	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. Nanoscale, 2021, 13, 5479-5488.	5.6	61
14	Quantum Dynamics Studies of the Significant Intramolecular Isotope Effects on the Nonadiabatic $Be \langle \sup \rangle \langle \sup \rangle \langle \sup \rangle P + HD \hat{\sigma}^+ BeH \langle \sup \rangle \langle \sup \rangle / BeD \langle \sup \rangle \langle \sup \rangle + D/H$ Reaction. Journal of Physical Chemistry A, 2021, 125, 235-242.	2.5	9
15	Feshbach resonances in $D \hat{\sigma}^+ \% + \hat{\sigma}^+ \% \langle \sup \rangle HD \langle \sup \rangle \langle i \rangle \nu \langle i \rangle \hat{\sigma}^+ \hat{\sigma}^+ 1, \langle i \rangle j \langle i \rangle \hat{\sigma}^+ \hat{\sigma}^+ 0$ reaction at low collision energies. Journal of Computational Chemistry, 2021, 42, 2334-2340.	3.3	1
16	Quantum Wave Packet Treatment of Cold Nonadiabatic Reactive Scattering at the State-To-State Level. Journal of Physical Chemistry A, 2021, 125, 10111-10120.	2.5	15
17	Temperature- and pressure-dependent rate coefficient measurement for the reaction of $CH \langle \sub \rangle 2 \langle \sub \rangle OO$ with $CH \langle \sub \rangle 3 \langle \sub \rangle CH \langle \sub \rangle 2 \langle \sub \rangle CHO$ . Physical Chemistry Chemical Physics, 2020, 22, 25869-25875.	2.8	8
18	Structures, stabilities and electronic properties of $Ti m Si \hat{\sigma}^+ n$ ( $m = \hat{\sigma}^+ \% 1 \hat{\sigma}^+ 2, n = \hat{\sigma}^+ \% 14 \hat{\sigma}^+ 20$ ) clusters: a combined ab initio and experimental study. European Physical Journal Plus, 2020, 135, 1.	2.6	14

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19	Competition between tubular, planar and cage geometries: a complete picture of structural evolution of $B_n$ ( $n = 31-50$ ) clusters. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12959-12966.	2.8	21
20	Theoretical study of surface-enhanced Raman scattering mechanism of scandium-doped copper/silver clusters. <i>Nanotechnology</i> , 2020, 31, 285201.	2.6	1
21	Quantum dynamics studies of isotope effects in the $Mg+(3p) + HD \rightarrow MgH/MgD + D/H$ insertion reaction. <i>Scientific Reports</i> , 2020, 10, 3410.	3.3	6
22	Dynamics study on the non-adiabatic $Na(3p) + HD \rightarrow NaH/NaD + D/H$ reaction: insertion-abstract mechanism. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 3633-3642.	2.8	10
23	Neural network potential energy surface and dynamical isotope effects for the $N_3 + H_2 \rightarrow NH_2 + N$ reaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22203-22214.	2.8	15
24	Ethanol and Acetaldehyde Decomposition on Co(0001): The Effect of Hydrogen Atom on C-O Bond Scission. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19045-19051.	3.1	4
25	Ultra-narrow electromagnetically induced transparency in the visible and near-infrared regions. <i>Applied Physics Letters</i> , 2019, 114, .	3.3	9
26	Biological nascent evolution of snail bone and collagen revealed by nonlinear optical microscopy. <i>Journal of Biophotonics</i> , 2019, 12, e201900119.	2.3	12
27	Methanol Decomposition on Co(0001): Influence of the Cobalt Oxidation State on Reactivity. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9139-9145.	3.1	6
28	Non-adiabatic state-to-state dynamic studies of $Na(3p) + H_2(v=1, 2, 3; j=0) \rightarrow NaH + H$ reactions. <i>Chemical Physics Letters</i> , 2019, 723, 128-132.	2.6	5
29	Acetaldehyde polymerization on Co(0001): the role of CO. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8275-8281.	2.8	0
30	Nonlinear optical characterization of porous carbon materials by CARS, SHG and TPEF. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 214, 58-66.	3.9	11
31	Diabatic potential energy surfaces of $MgH_2$ and dynamic studies for the $Mg(3p) + H_2 \rightarrow MgH + H$ reaction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6638-6647.	2.8	30
32	A global potential energy surface and time-dependent quantum wave packet calculation of $Au + H_2$ reaction. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25493.	2.0	14
33	Kinetics of the reaction of the simplest Criegee intermediate with ammonia: a combination of experiment and theory. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29669-29676.	2.8	27
34	New diabatic potential energy surfaces of the $NaH_2$ system and dynamics studies for the $Na(3p) + H_2 \rightarrow NaH + H$ reaction. <i>Scientific Reports</i> , 2018, 8, 17960.	3.3	16
35	Revisit of large-gap $Si_{16}$ clusters encapsulating group IV metal atoms (Ti, Zr, Hf). <i>Journal of Computational Chemistry</i> , 2018, 39, 2268-2272.	3.3	17
36	A new accurate potential energy surface for HeTiO system and rotational quenching of TiO due to He collisions. <i>Chemical Physics Letters</i> , 2018, 706, 323-327.	2.6	1

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37	Optical characterizations of two-dimensional materials using nonlinear optical microscopies of CARS, TPEF, and SHG. <i>Nanophotonics</i> , 2018, 7, 873-881.	6.0	35
38	Global diabatic potential energy surfaces for the $\text{BeH}_2$ system and dynamics studies on the $\text{Be}(\zeta^2\text{P}) + \text{H}_2(\text{X}^1\Sigma^+g) \hat{\text{a}}^+$ $\text{BeH}(\text{X}^1\Sigma^+g) + \text{H}(\text{X}^2\Sigma^+S)$ reaction. <i>RSC Advances</i> , 2018, 8, 22823-22834.	3.6	16
39	Advances in nonlinear optical microscopy for biophotonics. <i>Journal of Nanophotonics</i> , 2018, 12, 1.	1.0	24
40	Coupling effect on charge-transfer mechanism of surface-enhanced resonance Raman scattering. <i>Journal of Raman Spectroscopy</i> , 2017, 48, 560-569.	2.5	15
41	Structures and electronic properties of $\text{B}_3\text{Si}_n$ ( $n = 4-10$ ) clusters: A combined <i>ab initio</i> and experimental study. <i>Journal of Chemical Physics</i> , 2017, 146, 044306.	3.0	27
42	Theoretical investigations of the $\text{Au}^+ + \text{H}_2$ reactive scattering by the time-dependent quantum wave packet method. <i>International Journal of Modern Physics B</i> , 2017, 31, 1750039.	2.0	4
43	Global $\text{X}^2\text{A}^2$ potential energy surface of $\text{LiH}$ and quantum dynamics of $\text{H} + \text{Li}_2(\text{X}^1\Sigma^+g) \hat{\text{a}}^+$ $\text{Li} + \text{LiH}(\text{X}^1\Sigma^+g)$ reaction. <i>International Journal of Quantum Chemistry</i> , 2017, 117, e25380.		
44	A new potential energy surface for the ground state of the $\text{LiH}_2$ system and dynamic studies on $\text{LiH}(\text{X}^2\Sigma^+g) + \text{H}(\text{X}^2\Sigma^+S) \hat{\text{a}}^+$ $\text{Li}(\text{X}^1\Sigma^+g) + \text{H}_2(\text{X}^1\Sigma^+g)$ . <i>RSC Advances</i> , 2017, 7, 7008-7014.	3.6	11
45	A neural network potential energy surface for the $\text{NaH}_2$ system and dynamics studies on the $\text{H}(2S) + \text{NaH}(\text{X}^1\Sigma^+) \hat{\text{a}}^+$ $\text{Na}(2S) + \text{H}_2(\text{X}^1\Sigma^+g)$ reaction. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19873-19880.	2.8	14
46	Surface-enhanced Raman scattering of pyrazine on $\text{Au}_5\text{Al}_5$ bimetallic nanoclusters. <i>RSC Advances</i> , 2017, 7, 12170-12178.	3.6	8
47	SERRS and absorption spectra of pyridine on $\text{Au}_m\text{Ag}_n$ ( $m+n=6$ ) bimetallic nanoclusters: substrate composition and applied electric field effects. <i>Nanotechnology</i> , 2017, 28, 475201.	2.6	1
48	A global potential energy surface and dynamics study of the $\text{Au}^+ + \text{H}_2 \hat{\text{a}}^+$ $\text{H} + \text{AuH}$ reaction. <i>RSC Advances</i> , 2017, 7, 35648-35654.	3.6	1
49	Quantum rotational scattering of $\text{H}_2$ and its isotopologues with He. <i>Molecular Physics</i> , 2017, 115, 2442-2450.	1.7	8
50	Influence of rovibrational excitation on the non-diabatic state-to-state dynamics for the $\text{Li}(2p) + \text{H}_2 \hat{\text{a}}^+$ $\text{LiH} + \text{H}$ reaction. <i>Scientific Reports</i> , 2017, 7, 3084.	3.3	14
51	A new potential energy surface of $\text{LiHCl}$ system and dynamic studies for the $\text{Li}(2S) + \text{HCl}(\text{X}^1\Sigma^+) \hat{\text{a}}^+$ $\text{LiCl}(\text{X}^1\Sigma^+) + \text{H}(2S)$ reaction. <i>Journal of Chemical Physics</i> , 2016, 145, 234312.	3.0	13
52	Global diabatic potential energy surfaces and quantum dynamical studies for the $\text{Li}(2p) + \text{H}_2(\text{X}^1\Sigma^+g) \hat{\text{a}}^+$ $\text{LiH}(\text{X}^1\Sigma^+g) + \text{H}$ reaction. <i>Scientific Reports</i> , 2016, 6, 25083.	3.3	28
53	Ultrafast Dynamics of Plasmon-Exciton Interaction of Ag Nanowire- Graphene Hybrids for Surface Catalytic Reactions. <i>Scientific Reports</i> , 2016, 6, 32724.	3.3	106
54	A new potential energy surface for the $\text{H}_2\text{S}$ system and dynamics study on the $\text{S}(1D) + \text{H}_2(\text{X}^1\Sigma^+g)$ reaction. <i>Scientific Reports</i> , 2015, 5, 14594.	3.3	16

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55	Effect of aqueous and ambient atmospheric environments on plasmon-driven selective reduction reactions. <i>Scientific Reports</i> , 2015, 5, 10269.	3.3	22
56	Non-Born-Oppenheimer stereodynamics study for the $D^+ + H_2$ ( $v, j = 0$ ) reaction using coherent switching with decay of mixing method. <i>Canadian Journal of Chemistry</i> , 2015, 93, 764-768.	1.1	0
57	A new potential energy surface for the ground electronic state of the $LiH_2$ system, and dynamics studies on the $H_2 + LiH(X^1\Sigma^+ + \text{Li}^2S) + H_2(X^1\Sigma^+g + \text{Li}^2S)$ reaction. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 11732-11739.	2.8	47
58	Effect of Reagent Vibrational Excitation on the Dynamics of $F + H_2$ ( $v = 1, j = 0$ ) Reaction. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11111-11121.	2.5	11
59	Time-dependent quantum wave packet and quasiclassical trajectory studies of the $Au_2S + H_2(X^1\Sigma^+ + \text{AuH}(X^1\Sigma^+ + \text{H}_2S))$ reaction. <i>Molecular Physics</i> , 2014, 112, 2945-2953.	1.7	15
60	Charge transfer mechanism of SERS for metal-molecule-metal junction supported by graphene and boron-doped graphene. <i>RSC Advances</i> , 2014, 4, 63596-63602.	3.6	10
61	DFT study on the influence of electric field on surface-enhanced Raman scattering from pyridine-metal complex. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 62-67.	2.5	22
62	Molecular design of organic sensitizers absorbing over a broadened visible region for dye-sensitized solar cells. <i>RSC Advances</i> , 2014, 4, 57916-57922.	3.6	5
63	Time-dependent wave packet and quasiclassical trajectory studies of the $Au + HD$ reaction: competition between the reactive channels. <i>RSC Advances</i> , 2014, 4, 36189.	3.6	19
64	Ligand Desorption and Desulfurization on Silver Nanoparticles Using Sodium Borohydride in Water. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10509-10518.	3.1	21
65	State-Resolved Time-Dependent Wave Packet and Quasiclassical Trajectory Studies of the Adiabatic Reaction $S(3P) + HD$ on the ( $13A^3$ ) State. <i>Journal of Physical Chemistry A</i> , 2014, 118, 55-61.	2.5	10
66	Investigation of excited-state intramolecular proton transfer coupled charge transfer reaction of paeonol. <i>Canadian Journal of Chemistry</i> , 2014, 92, 274-278.	1.1	3
67	Visualized method of chemical enhancement mechanism on SERS and TERS. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 533-540.	2.5	107
68	TDDFT studies of electronic spectra and excited states of the triphenylamine-based organic sensitizers and organic sensitizer-titanium dioxide cluster complexes. <i>RSC Advances</i> , 2013, 3, 12133.	3.6	11
69	The impact of the number of layers of a graphene nanopore on DNA translocation. <i>Soft Matter</i> , 2013, 9, 960-966.	2.7	52
70	STUDY OF THE $S_1$ AND $S_2$ EXCITED STATES OF GAS-PHASE PROTONATED SCHIFF BASE RETINAL CHROMOPHORES IN ONE AND TWO PHOTON ABSORPTION. <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 121-132.	1.8	2
71	Theoretical studies of the stereodynamics for the reaction $H + LiH$ ( $v = 0, j = 0$ ) Reaction. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11111-11121.	1.7	22
72	Direct visual evidence for the chemical mechanism of surface-enhanced resonance Raman scattering via charge transfer. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 137-143.	2.5	79

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73	Direct visual evidence for the chemical mechanism of surface-enhanced resonance Raman scattering via charge transfer: (II) Binding-site and quantum-size effects. <i>Journal of Raman Spectroscopy</i> , 2009, 40, 1172-1177.	2.5	28
74	Theoretical study of electronic structure and excited states properties of two dyes for dye-sensitized solar cells. <i>Molecular Physics</i> , 2009, 107, 2569-2577.	1.7	6
75	Theoretical study on SERRS of rhodamine 6G adsorbed on Ag <sub>2</sub> cluster: chemical mechanism via intermolecular or intramolecular charge transfer. <i>Journal of Raman Spectroscopy</i> , 2008, 39, 1170-1177.	2.5	23
76	CONTROL OF SUCCESSIVELY SWITCHING FROM LLCT TO ILCT AND MLCT EXCITED STATES IN PLATINUM(II) TERPYRIDYL ACETYLIDE COMPLEXES BY SEQUENTIAL PROTONATIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 103-111.	1.8	3