

# 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	Visualized method of chemical enhancement mechanism on SERS and TERS. Journal of Raman Spectroscopy, 2014, 45, 533-540.	2.5	107
2	Ultrafast Dynamics of Plasmon-Exciton Interaction of Ag Nanowire- Graphene Hybrids for Surface Catalytic Reactions. Scientific Reports, 2016, 6, 32724.	3.3	106
3	Direct visual evidence for the chemical mechanism of surface-enhanced resonance Raman scattering via charge transfer. Journal of Raman Spectroscopy, 2009, 40, 137-143.	2.5	79
4	Accurate electronic properties and non-linear optical response of two-dimensional MA2Z4. Nanoscale, 2021, 13, 5479-5488.	5.6	61
5	The impact of the number of layers of a graphene nanopore on DNA translocation. Soft Matter, 2013, 9, 960-966.	2.7	52
6	A new potential energy surface for the ground electronic state of the $\text{LiH}^{2+}$ system, and dynamics studies on the $\text{H}^{2+} + \text{LiH}^{1+} \rightarrow \text{Li}^{2+} + \text{H}^{2+}$ reaction. Physical Chemistry Chemical Physics, 2015, 17, 11732-11739.	2.8	47
7	Optical characterizations of two-dimensional materials using nonlinear optical microscopies of CARS, TPEF, and SHG. Nanophotonics, 2018, 7, 873-881.	6.0	35
8	Diabatic potential energy surfaces of $\text{MgH}^{2+}$ and dynamic studies for the $\text{Mg}^{3+} + \text{H}^{2+} \rightarrow \text{MgH}^{2+} + \text{H}$ reaction. Physical Chemistry Chemical Physics, 2018, 20, 6638-6647.	2.8	30
9	Direct visual evidence for the chemical mechanism of surface-enhanced resonance Raman scattering via charge transfer: (II) Binding-site and quantum-size effects. Journal of Raman Spectroscopy, 2009, 40, 1172-1177.	2.5	28
10	Global diabatic potential energy surfaces and quantum dynamical studies for the $\text{Li}(2p) + \text{H}_2(X^{1\Sigma_g}) \rightarrow \text{LiH}(X^{1\Sigma_g}) + \text{H}$ reaction. Scientific Reports, 2016, 6, 25083.	3.3	28
11	Structures and electronic properties of $\text{B}_3\text{Si}_n^{+}$ ( $n = 4 \sim 10$ ) clusters: A combined <i>ab initio</i> and experimental study. Journal of Chemical Physics, 2017, 146, 044306.	3.0	27
12	Kinetics of the reaction of the simplest Criegee intermediate with ammonia: a combination of experiment and theory. Physical Chemistry Chemical Physics, 2018, 20, 29669-29676.	2.8	27
13	Advances in nonlinear optical microscopy for biophotonics. Journal of Nanophotonics, 2018, 12, 1.	1.0	24
14	Theoretical study on SERRS of rhodamine 6G adsorbed on $\text{Ag}^{2+}$ cluster: chemical mechanism via intermolecular or intramolecular charge transfer. Journal of Raman Spectroscopy, 2008, 39, 1170-1177.	2.5	23
15	Theoretical studies of the stereodynamics for the reaction $\text{H} + \text{LiH}^{+} (\langle i \rangle = 0, \langle j \rangle = 0)$ . <a href="#">Tj ETQq1 1 0,784314,rgBT /Over</a>	1.7	22
16	DFT study on the influence of electric field on surface-enhanced Raman scattering from pyridine-metal complex. Journal of Raman Spectroscopy, 2014, 45, 62-67.	2.5	22
17	Effect of aqueous and ambient atmospheric environments on plasmon-driven selective reduction reactions. Scientific Reports, 2015, 5, 10269.	3.3	22
18	Ligand Desorption and Desulfurization on Silver Nanoparticles Using Sodium Borohydride in Water. Journal of Physical Chemistry C, 2014, 118, 10509-10518.	3.1	21

#	ARTICLE	IF	CITATIONS
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	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
21	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
22	A new potential energy surface for the H <sub>2</sub> S system and dynamics study on the S(1D) + H <sub>2</sub> (X1 $\Sigma$ g <sup>+</sup> ) reaction. <i>Scientific Reports</i> , 2015, 5, 14594.	3.3	16
23	New diabatic potential energy surfaces of the NaH <sub>2</sub> system and dynamics studies for the Na(3p) + H <sub>2</sub> + NaH reaction. <i>Scientific Reports</i> , 2018, 8, 17960.	3.3	16
24	Global diabatic potential energy surfaces for the BeH <sub>2</sub> ( $\Sigma$ g <sup>+</sup> ) + H <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) + BeH <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) + H <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) + H <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) reaction. <i>RSC Advances</i> , 2018, 8, 22823-22834.	3.6	16
25	Time-dependent quantum wave packet and quasiclassical trajectory studies of the AuH(X $\Sigma$ g <sup>+</sup> ) + H <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) + AuH(X $\Sigma$ g <sup>+</sup> ) + H <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) reaction. <i>Molecular Physics</i> , 2014, 112, 2945-2953.	1.7	15
26	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
27	Neural network potential energy surface and dynamical isotope effects for the N <sub>2</sub> ( $\Sigma$ g <sup>+</sup> ) + H <sub>2</sub> (X $\Sigma$ g <sup>+</sup> ) + NH <sub>2</sub> ( $\Sigma$ g <sup>+</sup> ) + H reaction. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 22203-22214.	2.8	15
28	Quantum Wave Packet Treatment of Cold Nonadiabatic Reactive Scattering at the State-To-State Level. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10111-10120.	2.5	15
29	A neural network potential energy surface for the NaH <sub>2</sub> system and dynamics studies on the H(2S) + NaH(X1 $\Sigma$ g <sup>+</sup> ) + Na(2S) + H <sub>2</sub> (X1 $\Sigma$ g <sup>+</sup> ) reaction. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 19873-19880.	2.8	14
30	Influence of rovibrational excitation on the non-diabatic state-to-state dynamics for the Li(2p) + H <sub>2</sub> + LiH reaction. <i>Scientific Reports</i> , 2017, 7, 3084.	3.3	14
31	A global potential energy surface and time-dependent quantum wave packet calculation of AuH reaction. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25493.	2.0	14
32	Structures, stabilities and electronic properties of TimSi <sup>m</sup> (m = 1-2, n = 14-20) clusters: a combined ab initio and experimental study. <i>European Physical Journal Plus</i> , 2020, 135, 1.	2.6	14
33	A new potential energy surface of LiHCl system and dynamic studies for the Li(2S) + HCl(X1 $\Sigma$ g <sup>+</sup> ) + H(2S) reaction. <i>Journal of Chemical Physics</i> , 2016, 145, 234312.	3.0	13
34	Biological nascent evolution of snail bone and collagen revealed by nonlinear optical microscopy. <i>Journal of Biophotonics</i> , 2019, 12, e201900119.	2.3	12
35	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
36	Effect of Reagent Vibrational Excitation on the Dynamics of F + H <sub>2</sub> ( $v = 1, j = 1$ ) reaction. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10111-10120.	2.5	11

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37	A new potential energy surface for the ground state of the $\text{LiH}^2$ system and dynamic studies on $\text{Li}^2(\text{X}^2\text{I}^2) + \text{H}^2\text{S} \rightarrow \text{Li}^2(\text{S}) + \text{H}^2(\text{X}^1\text{I}^2\text{g})$ . RSC Advances, 2017, 7, 7008-7014.	3.6	11
38	Nonlinear optical characterization of porous carbon materials by CARS, SHG and TPEF. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 58-66.	3.9	11
39	Charge transfer mechanism of SERS for metal-molecule-metal junction supported by graphene and boron-doped graphene. RSC Advances, 2014, 4, 63596-63602.	3.6	10
40	State-Resolved Time-Dependent Wave Packet and Quasiclassical Trajectory Studies of the Adiabatic Reaction $\text{S}(3\text{P}) + \text{HD}$ on the $(13\text{A}^3)$ State. Journal of Physical Chemistry A, 2014, 118, 55-61.	2.5	10
41	Dynamics study on the non-adiabatic $\text{Na}(3\text{p}) + \text{HD} \rightarrow \text{NaH}/\text{NaD} + \text{D}/\text{H}$ reaction: insertion-abstracton mechanism. Physical Chemistry Chemical Physics, 2020, 22, 3633-3642.	2.8	10
42	Ultra-narrow electromagnetically induced transparency in the visible and near-infrared regions. Applied Physics Letters, 2019, 114, .	3.3	9
43	Quantum Dynamics Studies of the Significant Intramolecular Isotope Effects on the Nonadiabatic $\text{Be}^2(\text{P}) + \text{HD} \rightarrow \text{BeH}/\text{BeD} + \text{D}/\text{H}$ Reaction. Journal of Physical Chemistry A, 2021, 125, 235-242.	2.5	9
44	Surface-enhanced Raman scattering of pyrazine on $\text{Au}_5\text{Al}_5$ bimetallic nanoclusters. RSC Advances, 2017, 7, 12170-12178.	3.6	8
45	Quantum rotational scattering of $\text{H}_2$ and its isotopologues with He. Molecular Physics, 2017, 115, 2442-2450.	1.7	8
46	Temperature- and pressure-dependent rate coefficient measurement for the reaction of $\text{CH}_2\text{OO}$ with $\text{CH}_3\text{CH}_2\text{CHO}$ . Physical Chemistry Chemical Physics, 2020, 22, 25869-25875.	2.8	8
47	Dramatically Enhanced Second Harmonic Generation in Janus Group-III Chalcogenide Monolayers. Advanced Optical Materials, 2022, 10, .	7.3	8
48	Global $\text{X}^2$ potential energy surface of $\text{Li}_2\text{H}$ and quantum dynamics of $\text{H}^2\text{Li}_2(\text{X}^1\text{I}^2\text{g}) \rightarrow \text{Li}^2\text{H}(\text{X}^1\text{I}^2\text{g}) + \text{H}$ reaction. International Journal of Quantum Chemistry, 2017, 117, e25380.	2.8	7
49	Time-dependent wave packet dynamics study of the resonances in the $\text{H} + \text{LiH}^2$ ( $v=0$ ). Tj ETQq1 1 0.784314 rgBT Chemical Physics, 2022, 24, 15532-15539.	2.8	7
50	Theoretical study of electronic structure and excited states properties of two dyes for dye-sensitized solar cells. Molecular Physics, 2009, 107, 2569-2577.	1.7	6
51	Methanol Decomposition on $\text{Co}(0001)$ : Influence of the Cobalt Oxidation State on Reactivity. Journal of Physical Chemistry C, 2019, 123, 9139-9145.	3.1	6
52	Quantum dynamics studies of isotope effects in the $\text{Mg}^+(3\text{p}) + \text{HD} \rightarrow \text{MgH}^+/\text{MgD}^+ + \text{D}/\text{H}$ insertion reaction. Scientific Reports, 2020, 10, 3410.	3.3	6
53	Stereodynamics-Controlled Product Branching in the Nonadiabatic $\text{H} + \text{NaD} \rightarrow \text{Na}(3\text{s}, 3\text{p}) + \text{HD}$ Reaction at Low Temperatures. Journal of Physical Chemistry A, 2022, 126, 2453-2462.	2.5	6
54	Molecular design of organic sensitizers absorbing over a broadened visible region for dye-sensitized solar cells. RSC Advances, 2014, 4, 57916-57922.	3.6	5

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55	Non-adiabatic state-to-state dynamic studies of $\text{Na}(3p)\hat{A}^{-} + \hat{A}^{-}\text{H}_2(\hat{v}^{-} = \hat{A}^{-}1, 2, 3; \hat{j}^{-} = \hat{A}^{-}0)\hat{A}^{-}\hat{A}^{\dagger}\hat{A}^{-}\text{NaH}\hat{A}^{-} + \hat{A}^{-}\text{H}$ reactions. <i>Chemical Physics Letters</i> , 2019, 723, 128-132.	2.6	5
56	Transition metal-doped Bn ( $n\hat{A}^{-}\% = \hat{A}^{-}\%7\hat{A}^{-}10$ ) clusters: confirmation of a circular disk Jellium model. <i>European Physical Journal Plus</i> , 2021, 136, 1.	2.6	5
57	Evolution of Water Layer Adsorption on the GaN(0001) Surface and Its Influence on Electronic Properties. <i>Journal of Physical Chemistry C</i> , 2021, 125, 667-674.	3.1	5
58	Theoretical investigations of the $\text{Au}^{++}\text{H}\langle\text{sub}\rangle 2\langle\text{sub}\rangle$ reactive scattering by the time-dependent quantum wave packet method. <i>International Journal of Modern Physics B</i> , 2017, 31, 1750039.	2.0	4
59	Ethanol and Acetaldehyde Decomposition on Co(0001): The Effect of Hydrogen Atom on C $\hat{A}^{-}$ O Bond Scission. <i>Journal of Physical Chemistry C</i> , 2019, 123, 19045-19051.	3.1	4
60	Inelastic, exchange, and reactive processes in rovibrationally excited collisions of HD with H. <i>Monthly Notices of the Royal Astronomical Society</i> , 2021, 507, 6012-6019.	4.4	4
61	Representing globally accurate reactive potential energy surfaces with complex topography by combining Gaussian process regression and neural networks. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12827-12836.	2.8	4
62	Wave Packet Approach to Adiabatic and Nonadiabatic Dynamics of Cold Inelastic Scatterings. <i>Molecules</i> , 2022, 27, 2912.	3.8	4
63	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
64	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
65	STUDY OF THE $S\langle\text{sub}\rangle 1\langle\text{sub}\rangle$ AND $S\langle\text{sub}\rangle 2\langle\text{sub}\rangle$ 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
66	SERRS and absorption spectra of pyridine on $\text{Au}\langle\text{sub}\rangle m\langle\text{sub}\rangle / \text{Ag}\langle\text{sub}\rangle n\langle\text{sub}\rangle$ ( $\langle\text{sub}\rangle m\langle\text{sub}\rangle + \langle\text{sub}\rangle n\langle\text{sub}\rangle = 6$ ) bimetallic nanoclusters: substrate composition and applied electric field effects. <i>Nanotechnology</i> , 2017, 28, 475201.	2.6	1
67	A global potential energy surface and dynamics study of the $\text{Au}^{+} + \text{H}_2 \hat{A}^{\dagger} \text{H} + \text{Au} + \text{H}$ reaction. <i>RSC Advances</i> , 2017, 7, 35648-35654.	3.6	1
68	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
69	Theoretical study of surface-enhanced Raman scattering mechanism of scandium-doped copper/silver clusters. <i>Nanotechnology</i> , 2020, 31, 285201.	2.6	1
70	Time-dependent wave packet dynamics study of non-adiabatic $\text{Li}(2p)\hat{A}^{-} + \hat{A}^{-}\text{HD}\hat{A}^{\dagger}\hat{A}^{-}\text{LiH}/\text{LiD}\hat{A}^{-} + \hat{A}^{-}\text{H}$ reaction in a diabatic representation. <i>Chemical Physics Letters</i> , 2021, 764, 138279.	2.6	1
71	Non-adiabatic quantum dynamics studies of the $\text{Mg} + (3p)\hat{A}^{-} + \hat{A}^{-}\text{D}_2\hat{A}^{\dagger}\hat{A}^{-}\text{MgD} + \hat{A}^{-}\text{D}$ reaction. <i>Chemical Physics</i> , 2021, 550, 111311.	1.9	1
72	Feshbach resonances in $\text{D}\hat{A}^{-}\% + \hat{A}^{-}\% \langle\text{scp}\rangle \text{HD} \langle\text{scp}\rangle (\langle\text{sub}\rangle v\langle\text{sub}\rangle / \hat{A}^{-} = \hat{A}^{-}1, \langle\text{sub}\rangle j\langle\text{sub}\rangle / \hat{A}^{-} = \hat{A}^{-}0)$ reaction at low collision energies. <i>Journal of Computational Chemistry</i> , 2021, 42, 2334-2340.	3.3	1

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73	Non-adiabatic couplings induced complex-forming mechanism in $H+MgH+ \hat{\alpha}^+ Mg^{++}H_2$ reaction. Chinese Journal of Chemical Physics, 2022, 35, 345-352.	1.3	1
74	Non-Born-Oppenheimer stereodynamics study for the $D^+ + H_2$ ( $v, j = 0$ ) reaction using coherent switching with decay of mixing method. Canadian Journal of Chemistry, 2015, 93, 764-768.	1.1	0
75	Acetaldehyde polymerization on Co(0001): the role of CO. Physical Chemistry Chemical Physics, 2019, 21, 8275-8281.	2.8	0
76	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