Hua Guo

List of Publications by Year
in descending order

598 papers	35,688 citations	12597 71 h-index	6349 163 g-index
615 all docs	615 docs citations	615 times ranked	27101 citing authors

#	Article	IF	Citations
1	Dynamics in Heterogeneous and Single-Site Catalysis. , 2024, , 649-657.		0
2	Collisionâ€induced spinâ€orbit relaxation of highly vibrationally excited NO near 1 K. Natural Sciences, 2022, 2, e20210074.	1.0	5
3	Influence of supercell size on Gas-Surface Scattering: A case study of CO scattering from Au(1 1 1). Chemical Physics, 2022, 554, 111423.	0.9	11
4	Reaction Pathway Control via Reactant Vibrational Excitation and Impact on Product Vibrational Distributions: The O + HO₂ â†' OH + O₂ Atmospheric Reaction. Journal of Physical Chemistry Letters, 2022, 13, 1872-1878.	2.1	4
5	Stereodynamical Control of Cold Collisions of Polyatomic Molecules with Atoms. Journal of Physical Chemistry Letters, 2022, 13, 1777-1784.	2.1	11
6	Semiclassical Trajectory Studies of Reactive and Nonreactive Scattering of OH(A²Σ⁺) by H₂ Based on an Improved Fullâ€Dimensional Ab Initio Diabatic Potential Energy Matrix. ChemPhysChem, 2022, 23, .	1.0	7
7	Acetylene hydrogenation catalyzed by bare and Ni doped CeO₂(110): the role of frustrated Lewis pairs. Physical Chemistry Chemical Physics, 2022, 24, 11295-11304.	1.3	12
8	First-Principles Insights into Adiabatic and Nonadiabatic Vibrational Energy-Transfer Dynamics during Molecular Scattering from Metal Surfaces: The Importance of Surface Reactivity. Journal of Physical Chemistry Letters, 2022, 13, 3450-3461.	2.1	9
9	Full-dimensional quantum studies of vibrational energy transfer dynamics between H₂O and Ar: theory assessing experiment. Physical Chemistry Chemical Physics, 2022, 24, 13542-13549.	1.3	10
10	Mechanism and Dynamics of CO₂ Formation in Formic Acid Decomposition on Pt Surfaces. ACS Catalysis, 2022, 12, 6486-6494.	5.5	2
11	Differential Cross Sections for Cold, State-to-State Spinâ€“Orbit Changing Collisions of NO(v =) Tj ETQq1 1 0.784314 rgBT /Over	1.1	3
12	Internal conversion and intersystem crossing dynamics based on coupled potential energy surfaces with full geometry-dependent spinâ€“orbit and derivative couplings. Nonadiabatic photodissociation dynamics of NH₃(A) leading to the NH(X³Σ^{â^'}, a¹Δ") + H₂ channel. Physical Chemistry Chemical Physics, 2022, 24, 15060-15067.	1.3	3
13	Reactive and Nonreactive Collisions between NO(X²Π) and O(³P) under Hyperthermal Conditions. Journal of Physical Chemistry A, 2022, 126, 4277-4285.	1.1	5
14	Frustrated Lewis Pairs in Heterogeneous Catalysis: Theoretical Insights. Molecules, 2022, 27, 3734.	1.7	5
15	CO2 chemisorption and dissociation on flat and stepped transition metal surfaces. Applied Surface Science, 2022, 599, 154024.	3.1	11
16	Ultrasensitive small molecule fluorogenic probe for human heparanase. Chemical Science, 2021, 12, 239-246.	3.7	12
17	High-fidelity first principles nonadiabaticity: diabatization, analytic representation of global diabatic potential energy matrices, and quantum dynamics. Physical Chemistry Chemical Physics, 2021, 23, 24962-24983.	1.3	29
18	Quasiclassical simulations based on cluster models reveal vibration-facilitated roaming in the isomerization of CO adsorbed on NaCl. Nature Chemistry, 2021, 13, 249-254.	6.6	9

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19	Insights into the Formation of Hydroxyl Radicals with Nonthermal Vibrational Excitation in the Meinel Airglow. Journal of Physical Chemistry Letters, 2021, 12, 1822-1828.	2.1	5
20	Insights into adsorption, diffusion, and reactions of atomic nitrogen on a highly oriented pyrolytic graphite surface. Journal of Chemical Physics, 2021, 154, 074708.	1.2	5
21	Single atom catalysis poised to transition from an academic curiosity to an industrially relevant technology. Nature Communications, 2021, 12, 895.	5.8	52
22	Potential energy surfaces for high-energy N + O2 collisions. Journal of Chemical Physics, 2021, 154, 084304.	1.2	23
23	Enabling complete multichannel nonadiabatic dynamics: A global representation of the two-channel coupled, 1,21A and 13A states of NH3 using neural networks. Journal of Chemical Physics, 2021, 154, 094121.	1.2	19
24	Rainbow scattering in rotationally inelastic collisions of HCl and H2. Journal of Chemical Physics, 2021, 154, 104304.	1.2	2
25	High-Efficiency Water Gas Shift Reaction Catalysis on Î±-MoC Promoted by Single-Atom Ir Species. ACS Catalysis, 2021, 11, 5942-5950.	5.5	65
26	Direct Dynamics Simulations of Hyperthermal O(3P) Collisions with Pristine, Defected, Oxygenated, and Nitridated Graphene Surfaces. Journal of Physical Chemistry C, 2021, 125, 9795-9808.	1.5	10
27	Precision test of statistical dynamics with state-to-state ultracold chemistry. Nature, 2021, 593, 379-384.	13.7	53
28	Vibrational energy levels of the S ₀ and S ₁ states of formaldehyde using an accurate ab initio based global diabatic potential energy matrix. Molecular Physics, 2021, 119, .	0.8	3
29	Enabling a Unified Description of Both Internal Conversion and Intersystem Crossing in Formaldehyde: A Global Coupled Quasi-Diabatic Hamiltonian for Its S₀, S₁, and T₁ States. Journal of Chemical Theory and Computation, 2021, 17, 4157-4168.	2.3	12
30	Rotational Modulation of Ãƒ2Aâ€³-State Photodissociation of HCO via Rennerâ€“Teller Nonadiabatic Transitions. Journal of Physical Chemistry Letters, 2021, 12, 6582-6588.	2.1	7
31	Unraveling the Intermediate Reaction Complexes and Critical Role of Support-Derived Oxygen Atoms in CO Oxidation on Single-Atom Pt/CeO₂. ACS Catalysis, 2021, 11, 8701-8715.	5.5	51
32	Full-Dimensional Global Potential Energy Surface for the KRb + KRb â†' K₂Rb₂* â†' K₂ + Rb₂ Reaction with Accurate Long-Range Interactions and Quantum Statistical Calculation of the Product State Distribution under Ultracold Conditions. Journal of Physical Chemistry A, 2021, 125, 6198-6206.	1.1	3
33	The puzzle of rapid hydrogen oxidation on Pt(111). Molecular Physics, 2021, 119, .	0.8	7
34	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of OH(A2Î£+) by H2. Nature Chemistry, 2021, 13, 909-915.	6.6	17
35	A Time-Independent Quantum Approach to Ro-vibrationally Inelastic Scattering between Atoms and Triatomic Molecules. Journal of Physical Chemistry A, 2021, 125, 6864-6871.	1.1	8
36	Quantum dynamics with ab initio potentials. Journal of Chemical Physics, 2021, 155, 080401.	1.2	2

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37	Dynamics of Initial Hydrogen Spillover from a Single Atom Platinum Active Site to the Cu(111) Host Surface: The Impact of Substrate Electronâ€“Hole Pairs. Journal of Physical Chemistry Letters, 2021, 12, 8423-8429.	2.1	19
38	Determining reaction pathways at low temperatures by isotopic substitution: the case of BeD⁺ + H₂O. New Journal of Physics, 2021, 23, 115004.	1.2	4
39	Vibrational mode-specificity in the dynamics of the Cl + C2H6 â†' HCl + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 114303.	1.2	14
40	Towards bridging the structure gap in heterogeneous catalysis: the impact of defects in dissociative chemisorption of methane on Ir surfaces. Physical Chemistry Chemical Physics, 2021, 23, 4376-4385.	1.3	31
41	Theoretical H + O₃ rate coefficients from ring polymer molecular dynamics on an accurate global potential energy surface: assessing experimental uncertainties. Physical Chemistry Chemical Physics, 2021, 23, 3300-3310.	1.3	4
42	Isomer-specific kinetics of the C ⁺ + H ₂ O reaction at the temperature of interstellar clouds. Science Advances, 2021, 7, .	4.7	16
43	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
44	Engineering catalyst supports to stabilize PdOx two-dimensional rafts for water-tolerant methane oxidation. Nature Catalysis, 2021, 4, 830-839.	16.1	86
45	Full-Dimensional Potential Energy Surface for Ro-vibrationally Inelastic Scattering between H₂ Molecules. Journal of Chemical Theory and Computation, 2021, 17, 6747-6756.	2.3	11
46	Infrared Activities of Adsorbed Species on Metal Surfaces: The Puzzle of Adsorbed Methyl (CH3). Journal of Physical Chemistry Letters, 2021, 12, 11164-11169.	2.1	0
47	Orbiting resonances in formaldehyde reveal coupling of roaming, radical, and molecular channels. Science, 2021, 374, 1122-1127.	6.0	15
48	Quantum Wave Packet Treatment of Cold Nonadiabatic Reactive Scattering at the State-To-State Level. Journal of Physical Chemistry A, 2021, 125, 10111-10120.	1.1	15
49	Assessing density functionals for describing methane dissociative chemisorption on Pt(110)-(2Ã—1) surface. Chinese Journal of Chemical Physics, 2021, 34, 883-895.	0.6	2
50	Environmentally benign synthesis of a PGM-free catalyst for low temperature CO oxidation. Applied Catalysis B: Environmental, 2020, 264, 118547.	10.8	20
51	Extending the Representation of Multistate Coupled Potential Energy Surfaces To Include Properties Operators Using Neural Networks: Application to the 1,2¹A States of Ammonia. Journal of Chemical Theory and Computation, 2020, 16, 302-313.	2.3	39
52	Insights into the Mechanism of Nonadiabatic Photodissociation from Product Vibrational Distributions. The Remarkable Case of Phenol. Journal of Physical Chemistry Letters, 2020, 11, 191-198.	2.1	25
53	Impact of Diabolical Singular Points on Nonadiabatic Dynamics and a Remedy: Photodissociation of Ammonia in the First Band. Journal of Chemical Theory and Computation, 2020, 16, 6776-6784.	2.3	6
54	Photo-excitation of long-lived transient intermediates in ultracold reactions. Nature Physics, 2020, 16, 1132-1136.	6.5	76

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55	Theoretical Investigations of Rate Coefficients for H + O3and HO2+ O Reactions on a Full-Dimensional Potential Energy Surface. Journal of Physical Chemistry A, 2020, 124, 6427-6437.	1.1	16
56	Neural Network Based Quasi-diabatic Representation for S₀ and S₁ States of Formaldehyde. Journal of Physical Chemistry A, 2020, 124, 10132-10142.	1.1	21
57	Exploring reactivity and product formation in N(4S) collisions with pristine and defected graphene with direct dynamics simulations. Journal of Chemical Physics, 2020, 153, 184702.	1.2	13
58	Dynamics studies of diglycine scattering from highly oriented pyrolytic graphite. Chinese Journal of Chemical Physics, 2020, 33, 196-202.	0.6	3
59	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
60	Origin of the â€œoddâ€•behavior in the ultraviolet photochemistry of ozone. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 21065-21069.	3.3	10
61	Potential Energy Landscape of CO Adsorbates on NaCl(100) and Implications in Isomerization of Vibrationally Excited CO. Journal of Physical Chemistry C, 2020, 124, 19146-19156.	1.5	12
62	Advances and New Challenges to Bimolecular Reaction Dynamics Theory. Journal of Physical Chemistry Letters, 2020, 11, 8844-8860.	2.1	46
63	Spectroscopic identification of the â€¢SSNO isomers. Journal of Chemical Physics, 2020, 153, 094303.	1.2	3
64	Following the microscopic pathway to adsorption through chemisorption and physisorption wells. Science, 2020, 369, 1461-1465.	6.0	42
65	Time-independent quantum theory on vibrational inelastic scattering between atoms and open-shell diatomic molecules: Applications to NO + Ar and NO + H scattering. Journal of Chemical Physics, 2020, 153, 144306.	1.2	13
66	Origin of Confined Catalysis in Nanoscale Reactors between Two-Dimensional Covers and Metal Substrates: Mechanical or Electronic?. Journal of Physical Chemistry C, 2020, 124, 11564-11573.	1.5	14
67	State-to-state scattering of highly vibrationally excited NO at broadly tunable energies. Nature Chemistry, 2020, 12, 528-534.	6.6	20
68	Nonadiabatic Electronic Energy Transfer in the Chemical Oxygenâ€“Iodine Laser: Powered by Derivative Coupling or Spinâ€“Orbit Coupling?. Journal of Physical Chemistry Letters, 2020, 11, 4768-4773.	2.1	10
69	On the nonadiabatic collisional quenching of OH(A) by H₂: a four coupled quasi-diabatic state description. Physical Chemistry Chemical Physics, 2020, 22, 13516-13527.	1.3	15
70	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
71	A Global Full-Dimensional Potential Energy Surface for the K₂Rb₂ Complex and Its Lifetime. Journal of Physical Chemistry Letters, 2020, 11, 2605-2610.	2.1	17
72	Mechanistic Insights into Photocatalyzed H₂ Dissociation on Au Clusters. Journal of the American Chemical Society, 2020, 142, 13090-13101.	6.6	48

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73	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
74	Statistical quantum mechanical approach to diatomâ€“diatom capture dynamics and application to ultracold KRb + KRb reaction. Journal of Chemical Physics, 2020, 152, 241103.	1.2	19
75	New Perspectives on CO₂â€“Pt(111) Interaction with a High-Dimensional Neural Network Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 5174-5181.	1.5	37
76	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
77	Stereodynamic control of overlapping resonances in cold molecular collisions. Physical Review Research, 2020, 2, .	1.3	14
78	Comprehensive Investigations of the Clâ€‰+â€‰CH ₃ OHâ€‰â†'â€‰HClâ€‰+â€‰CH ₃ O/CH <sub>2</ OH Reaction: Validation of Experiment and Dynamic Insights. CCS Chemistry, 2020, 2, 882-894.	4.6	36
79	Stereodynamical Control of a Quantum Scattering Resonance in Cold Molecular Collisions. Physical Review Letters, 2019, 123, 043401.	2.9	32
80	Dissociative Chemisorption of Methane on Stepped Ir(332) Surface: Density Functional Theory and Ab Initio Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 20893-20902.	1.5	12
81	The JPC Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
82	The JPC Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
83	Stereodynamical control of product branching in multi-channel barrierless hydrogen abstraction of CH₃OH by F. Chemical Science, 2019, 10, 7994-8001.	3.7	24
84	The JPC Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2
85	On the mechanism of alkyne hydrogenation catalyzed by Ga-doped ceria. Journal of Catalysis, 2019, 375, 410-418.	3.1	43
86	Globally Accurate Full-Dimensional Potential Energy Surface for H₂ + HCl Inelastic Scattering. Journal of Physical Chemistry A, 2019, 123, 6578-6586.	1.1	10
87	Breakdown of energy transfer gap laws revealed by full-dimensional quantum scattering between HF molecules. Nature Communications, 2019, 10, 4658.	5.8	17
88	Hot-electron effects during reactive scattering of H₂ from Ag(111): the interplay between mode-specific electronic friction and the potential energy landscape. Chemical Science, 2019, 10, 1089-1097.	3.7	35
89	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
90	Hot electron effects during reactive scattering of H₂ from Ag(111): assessing the sensitivity to initial conditions, coupling magnitude, and electronic temperature. Faraday Discussions, 2019, 214, 105-121.	1.6	15

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91	Dissection of the multichannel reaction of acetylene with atomic oxygen: from the global potential energy surface to rate coefficients and branching dynamics. Physical Chemistry Chemical Physics, 2019, 21, 1408-1416.	1.3	7
92	Diabatic and adiabatic representations: Electronic structure caveats. Computational and Theoretical Chemistry, 2019, 1152, 41-52.	1.1	15
93	Up to a Sign. The Insidious Effects of Energetically Inaccessible Conical Intersections on Unimolecular Reactions. Accounts of Chemical Research, 2019, 52, 501-509.	7.6	39
94	Mechanistic details of the MnO+ + H2/D2 reaction through temperature-dependent kinetics and statistical modeling. International Journal of Mass Spectrometry, 2019, 435, 26-33.	0.7	5
95	Scattering Dynamics of Glycine, H2O, and CO2 on Highly Oriented Pyrolytic Graphite. Journal of Physical Chemistry C, 2019, 123, 3605-3621.	1.5	7
96	Isotope-selective chemistry in the Be⁺(²S_{1/2}) + HOD â†' BeOD⁺/BeOH⁺ + H/D reaction. Physical Chemistry Chemical Physics, 2019, 21, 14005-14011.	1.3	14
97	First-principles dynamics of collisional intersystem crossing: resonance enhanced quenching of C(¹D) by N₂. Physical Chemistry Chemical Physics, 2019, 21, 8645-8653.	1.3	9
98	Competition between Proton Transfer and Proton Isomerization in the N₂ + HOC⁺ Reaction on an Ab Initio-Based Global Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 5347-5355.	1.1	6
99	Neural network based quasi-diabatic Hamiltonians with symmetry adaptation and a correct description of conical intersections. Journal of Chemical Physics, 2019, 150, 214101.	1.2	38
100	Quantum Stereodynamics of H₂ Scattering from Co(0001): Influence of Reaction Channels. Journal of Physical Chemistry C, 2019, 123, 16223-16231.	1.5	8
101	Anab initiobased full-dimensional potential energy surface for OH + O2â‡„ HO3and low-lying vibrational levels of HO3. Physical Chemistry Chemical Physics, 2019, 21, 13766-13775.	1.3	10
102	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
103	A Quasi-Diabatic Representation of the 1,2¹A States of Methylamine. Journal of Physical Chemistry A, 2019, 123, 5231-5241.	1.1	19
104	Au₂⁺ cannot catalyze conversion of methane to ethene at low temperature. Catalysis Science and Technology, 2019, 9, 2767-2780.	2.1	13
105	Dynamics in reactions on metal surfaces: A theoretical perspective. Journal of Chemical Physics, 2019, 150, 180901.	1.2	56
106	Bond dissociation energy of Au2+: A guided ion beam and theoretical investigation. Journal of Chemical Physics, 2019, 150, 174305.	1.2	9
107	Absorption Spectra of Acetylene, Vinylidene, and Their Deuterated Isotopologues on Ab Initio Potential Energy and Dipole Moment Surfaces. Journal of Physical Chemistry A, 2019, 123, 4232-4240.	1.1	7
108	Differential Cross Sections for State-to-State Collisions of NO(v = 10) in Near-Copropagating Beams. Journal of Physical Chemistry Letters, 2019, 10, 2422-2427.	2.1	17

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109	Origin of Thermal and Hyperthermal CO₂ from CO Oxidation on Pt Surfaces: The Role of Postâ€Transitionâ€State Dynamics, Active Sites, and Chemisorbed CO₂. Angewandte Chemie, 2019, 131, 6990-6994.	1.6	7
110	Diffraction of CH₄ from a Metal Surface. Journal of Physical Chemistry Letters, 2019, 10, 1574-1580.	2.1	12
111	Origin of Thermal and Hyperthermal CO₂ from CO Oxidation on Pt Surfaces: The Role of Postâ€Transitionâ€State Dynamics, Active Sites, and Chemisorbed CO₂. Angewandte Chemie - International Edition, 2019, 58, 6916-6920.	7.2	31
112	Accurate characterization of the lowest triplet potential energy surface of SO2 with a coupled cluster method. Journal of Chemical Physics, 2019, 150, 144303.	1.2	2
113	Viewpoint: New Physical Insights from Kinetics Studies. Journal of Physical Chemistry A, 2019, 123, 3057-3057.	1.1	4
114	Steric Effects in CO Oxidation on Pt(111) by Impinging Oxygen Atoms Lead to an Exclusive Hot Atom Mechanism. Journal of Physical Chemistry C, 2019, 123, 10509-10516.	1.5	8
115	Stabilizing High Metal Loadings of Thermally Stable Platinum Single Atoms on an Industrial Catalyst Support. ACS Catalysis, 2019, 9, 3978-3990.	5.5	233
116	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
117	Nonadiabatic Dynamics in Photodissociation of Hydroxymethyl in the 32A(3px) Rydberg State: A Nine-Dimensional Quantum Study. Journal of Physical Chemistry A, 2019, 123, 1937-1944.	1.1	8
118	Adiabatic and nonadiabatic energy dissipation during scattering of vibrationally excited CO from Au(111). Physical Review B, 2019, 100, .	1.1	23
119	Unexpected Indirect Dynamics in Base-Induced Elimination. Journal of the American Chemical Society, 2019, 141, 20300-20308.	6.6	19
120	Dynamical interference in the vibronic bond breaking reaction of HCO. Science Advances, 2019, 5, eaau0582.	4.7	15
121	Synthesis of Nickelâ€Doped Ceria Catalysts for Selective Acetylene Hydrogenation. ChemCatChem, 2019, 11, 1526-1533.	1.8	30
122	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2019, 123, 2287-2299.	1.5	30
123	Highly Localized SERS Measurements Using Single Silicon Nanowires Decorated with DNA Origami-Based SERS Probe. Nano Letters, 2019, 19, 1061-1066.	4.5	34
124	Representation of coupled adiabatic potential energy surfaces using neural network based quasi-diabatic Hamiltonians: 1,2 ²Aâ€² states of LiFH. Physical Chemistry Chemical Physics, 2019, 21, 14205-14213.	1.3	45
125	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
126	The near-UV absorber OSSO and its isomers. Chemical Communications, 2018, 54, 4517-4520.	2.2	18

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127	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
128	State-to-state quantum dynamics of the Hâ€¯+â€¯LiFâ€¯â†'â€¯Liâ€¯+â€¯HF reaction on an accurate ab initio potential energy surface. Chemical Physics, 2018, 515, 427-433.	0.9	3
129	First-Principles Insights into Ammonia Decomposition Catalyzed by Ru Clusters Anchored on Carbon Nanotubes: Size Dependence and Interfacial Effects. Journal of Physical Chemistry C, 2018, 122, 9091-9100.	1.5	35
130	Quantum dynamics of ClH2Oâ¯ photodetachment: Isotope effect and impact of anion vibrational excitation. Journal of Chemical Physics, 2018, 148, 064305.	1.2	4
131	A new potential energy surface and state-to-state quantum dynamics of the Liâ€â€+â€â€HFâ€â†'â€Hâ€â€+â€â€LiF reaction. Chemical Physics, 2018, 509, 66-71.	0.9	5
132	Autodetachment from Vibrationally Excited Vinylidene Anions. Journal of Physical Chemistry Letters, 2018, 9, 1058-1063.	2.1	15
133	Active vs. spectator modes in nonadiabatic photodissociation dynamics of the hydroxymethyl radical via the 22A(3s) Rydberg state. Journal of Chemical Physics, 2018, 148, 044305.	1.2	11
134	Probing the rate-determining region of the potential energy surface for a prototypical ionâ€“molecule reaction. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170146.	1.6	2
135	Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. Journal of the American Chemical Society, 2018, 140, 1986-1989.	6.6	42
136	Ab initio molecular dynamics study of the Eley-Rideal reaction of H + Clâ€“Au(111) â†' HCl + Au(111): Impact of energy dissipation to surface phonons and electron-hole pairs. Journal of Chemical Physics, 2018, 148, 014702.	1.2	25
137	Constructing High-Dimensional Neural Network Potential Energy Surfaces for Gasâ€“Surface Scattering and Reactions. Journal of Physical Chemistry C, 2018, 122, 1761-1769.	1.5	78
138	State-to-state mode specificity in H + DOH(Î½OH = 1) â†' HD + OH(Î½2 = 0) reaction: vibrational non-adiabaticity or local-mode excitation?. Physical Chemistry Chemical Physics, 2018, 20, 191-198.	1.3	12
139	Capture of SO₃isomers in the oxidation of sulfur monoxide with molecular oxygen. Chemical Communications, 2018, 54, 1690-1693.	2.2	19
140	Modified Gaussian Wave Packet Method for Calculating Initial State Wave Functions in Photodissociation. Journal of Chemical Theory and Computation, 2018, 14, 5527-5534.	2.3	3
141	Permutation invariant polynomial neural network approach to fitting potential energy surfaces. IV. Coupled diabatic potential energy matrices. Journal of Chemical Physics, 2018, 149, 144107.	1.2	61
142	Design of Effective Catalysts for Selective Alkyne Hydrogenation by Doping of Ceria with a Single-Atom Promotor. Journal of the American Chemical Society, 2018, 140, 12964-12973.	6.6	204
143	Correlating DFT Calculations with CO Oxidation Reactivity on Ga-Doped Pt/CeO₂ Single-Atom Catalysts. Journal of Physical Chemistry C, 2018, 122, 22460-22468.	1.5	91
144	Unraveling the Stereodynamics of Cold Controlled <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>HD</mml:mi><mml:mtext>â¯'</mml:mtext><mml:msub><mml:mrow><mml:mi mathvariant="normal">H</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:m Collisions. Physical Review Letters, 2018, 121, 113401.	2.9	39

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145	Dissociative Chemisorption of O₂ on Al(111): Dynamics on a Correlated Wave-Function-Based Potential Energy Surface. Journal of Physical Chemistry Letters, 2018, 9, 3271-3277.	2.1	40
146	Low temperature rates for key steps of interstellar gas-phase water formation. Science Advances, 2018, 4, eaar3417.	4.7	19
147	Communication: Fingerprints of reaction mechanisms in product distributions: Eley-Rideal-type reactions between D and CD3/Cu(111). Journal of Chemical Physics, 2018, 149, 031101.	1.2	16
148	Stretching vibration is a spectator in nucleophilic substitution. Science Advances, 2018, 4, eaas9544.	4.7	37
149	Influence of Rennerâ€“Teller Coupling between Electronic States on H + CO Inelastic Scattering. Journal of Physical Chemistry A, 2018, 122, 6381-6390.	1.1	4
150	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. ACS Nano, 2018, 12, 8415-8422.	7.3	75
151	Single atom detachment from Cu clusters, and diffusion and trapping on CeO₂(111): implications in Ostwald ripening and atomic redispersion. Nanoscale, 2018, 10, 17893-17901.	2.8	47
152	Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). Journal of Chemical Physics, 2018, 149, 044703.	1.2	15
153	Selective hydrogenation of 1,3-butadiene catalyzed by a single Pd atom anchored on graphene: the importance of dynamics. Chemical Science, 2018, 9, 5890-5896.	3.7	55
154	Fermi resonance controlled product branching in the H + HOD reaction. Physical Chemistry Chemical Physics, 2018, 20, 17029-17037.	1.3	16
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