Hua Guo

List of Publications by Year
in descending order

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178	4,687	94433	144013
papers	citations	37 h-index	57 g-index

186	186	186	5093
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High sulfur loading composite wrapped by 3D nitrogen-doped graphene as a cathode material for lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2014, 2, 5018-5023.	10.3	249
2	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.	13.7	204
3	Optimized Temperature Effect of Liâ€ion Diffusion with Layer Distance in Li(Ni_xMn_yCo_z)O₂ Cathode Materials for High Performance Liâ€ion Battery. Advanced Energy Materials, 2016, 6, 1501309.	19.5	182
4	3Dâ€Printed Cathodes of LiMn_{1â^'}_xFe_xPO₄ Nanocrystals Achieve Both Ultrahigh Rate and High Capacity for Advanced Lithiumâ€ion Battery. Advanced Energy Materials, 2016, 6, 1600856.	19.5	157
5	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.	4.6	127
6	High-Dimensional Atomistic Neural Network Potentials for Moleculeâ€“Surface Interactions: HCl Scattering from Au(111). Journal of Physical Chemistry Letters, 2017, 8, 666-672.	4.6	94
7	Correlating DFT Calculations with CO Oxidation Reactivity on Ga-Doped Pt/CeO₂ Single-Atom Catalysts. Journal of Physical Chemistry C, 2018, 122, 22460-22468.	3.1	91
8	Janus Solidâ€“Liquid Interface Enabling Ultrahigh Charging and Discharging Rate for Advanced Lithium-Ion Batteries. Nano Letters, 2015, 15, 6102-6109.	9.1	90
9	Control of chemical reactivity by transition-state and beyond. Chemical Science, 2016, 7, 3992-4003.	7.4	78
10	Constructing High-Dimensional Neural Network Potential Energy Surfaces for Gasâ€“Surface Scattering and Reactions. Journal of Physical Chemistry C, 2018, 122, 1761-1769.	3.1	78
11	A coreâ€“shell nanohollow-Î³-Fe₂O₃@graphene hybrid prepared through the Kirkendall process as a high performance anode material for lithium ion batteries. Chemical Communications, 2015, 51, 7855-7858.	4.1	76
12	Photo-excitation of long-lived transient intermediates in ultracold reactions. Nature Physics, 2020, 16, 1132-1136.	16.7	76
13	Plasmonic Hot-Carrier-Mediated Tunable Photochemical Reactions. ACS Nano, 2018, 12, 8415-8422.	14.6	75
14	Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes. Journal of Physical Chemistry A, 2017, 121, 2552-2557.	2.5	72
15	Permutation invariant polynomial neural network approach to fitting potential energy surfaces. IV. Coupled diabatic potential energy matrices. Journal of Chemical Physics, 2018, 149, 144107.	3.0	61
16	Dynamics in reactions on metal surfaces: A theoretical perspective. Journal of Chemical Physics, 2019, 150, 180901.	3.0	56
17	Encoding of vinylidene isomerization in its anion photoelectron spectrum. Science, 2017, 358, 336-339.	12.6	55
18	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.	7.4	55

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19	Excess Li-Ion Storage on Reconstructed Surfaces of Nanocrystals To Boost Battery Performance. Nano Letters, 2017, 17, 6018-6026.	9.1	53
20	Precision test of statistical dynamics with state-to-state ultracold chemistry. Nature, 2021, 593, 379-384.	27.8	53
21	Single atom catalysis poised to transition from an academic curiosity to an industrially relevant technology. Nature Communications, 2021, 12, 895.	12.8	52
22	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.	11.2	51
23	Mechanistic Insights into Photocatalyzed H₂ Dissociation on Au Clusters. Journal of the American Chemical Society, 2020, 142, 13090-13101.	13.7	48
24	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.	5.6	47
25	Advances and New Challenges to Bimolecular Reaction Dynamics Theory. Journal of Physical Chemistry Letters, 2020, 11, 8844-8860.	4.6	46
26	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.	2.8	45
27	On the mechanism of alkyne hydrogenation catalyzed by Ga-doped ceria. Journal of Catalysis, 2019, 375, 410-418.	6.2	43
28	Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. Journal of the American Chemical Society, 2018, 140, 1986-1989.	13.7	42
29	A Novel Class of Injectable Bioceramics That Glue Tissues and Biomaterials. Materials, 2018, 11, 2492.	2.9	42
30	Following the microscopic pathway to adsorption through chemisorption and physisorption wells. Science, 2020, 369, 1461-1465.	12.6	42
31	Soft-contact conductive carbon enabling depolarization of LiFePO4 cathodes to enhance both capacity and rate performances of lithium ion batteries. Journal of Power Sources, 2016, 331, 232-239.	7.8	41
32	Ab Initio Molecular Dynamics Study of Dissociative Chemisorption and Scattering of CO₂ on Ni(100): Reactivity, Energy Transfer, Steering Dynamics, and Lattice Effects. Journal of Physical Chemistry C, 2017, 121, 5594-5602.	3.1	41
33	Dissociative chemisorption of methane on Ni(111) using a chemically accurate fifteen dimensional potential energy surface. Physical Chemistry Chemical Physics, 2017, 19, 30540-30550.	2.8	40
34	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.	4.6	40
35	Many-Body Permutationally Invariant Polynomial Neural Network Potential Energy Surface for N₄. Journal of Chemical Theory and Computation, 2020, 16, 4822-4832.	5.3	40
36	Up to a Sign. The Insidious Effects of Energetically Inaccessible Conical Intersections on Unimolecular Reactions. Accounts of Chemical Research, 2019, 52, 501-509.	15.6	39

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37	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.	5.3	39
38	Neural network based quasi-diabatic Hamiltonians with symmetry adaptation and a correct description of conical intersections. Journal of Chemical Physics, 2019, 150, 214101.	3.0	38
39	Stretching vibration is a spectator in nucleophilic substitution. Science Advances, 2018, 4, eaas9544.	10.3	37
40	Optical Control of Reactions between Water and Laser-Cooled Be⁺ Ions. Journal of Physical Chemistry Letters, 2018, 9, 3555-3560.	4.6	37
41	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.	3.1	37
42	Dynamics of transient speciesviaanion photodetachment. Chemical Society Reviews, 2017, 46, 7650-7667.	38.1	35
43	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.	3.1	35
44	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.	7.4	35
45	Constructive and Destructive Interference in Nonadiabatic Tunneling via Conical Intersections. Journal of Chemical Theory and Computation, 2017, 13, 1902-1910.	5.3	34
46	Highly Localized SERS Measurements Using Single Silicon Nanowires Decorated with DNA Origami-Based SERS Probe. Nano Letters, 2019, 19, 1061-1066.	9.1	34
47	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.	13.7	33
48	Storage and Effective Migration of Li-Ion for Defected Î²-LiFePO₄ Phase Nanocrystals. Nano Letters, 2016, 16, 601-608.	9.1	31
49	Potential energy surface stationary points and dynamics of the F^{â^'}+ CH₃I double inversion mechanism. Physical Chemistry Chemical Physics, 2017, 19, 20127-20136.	2.8	31
50	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.	13.8	31
51	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.	2.8	31
52	Formation of mono/bi-layer iron phosphate and nucleation of LiFePO 4 nano-crystals from amorphous 2D sheets in charge/discharge process for cathode in high-performance Li-ion batteries. Nano Energy, 2015, 18, 187-195.	16.0	30
53	Reactive and Nonreactive Scattering of HCl from Au(111): An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry C, 2019, 123, 2287-2299.	3.1	30
54	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.	2.8	29

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55	Non-Adiabatic Effects on Excited States of Vinylidene Observed with Slow Photoelectron Velocity-Map Imaging. Journal of the American Chemical Society, 2016, 138, 16417-16425.	13.7	28
56	On the incorporation of the geometric phase in general single potential energy surface dynamics: A removable approximation to ab initio data. Journal of Chemical Physics, 2016, 145, 234111.	3.0	25
57	Controllable synthesis of LiFePO₄in different polymorphs and study of the reaction mechanism. Journal of Materials Chemistry A, 2017, 5, 14294-14300.	10.3	25
58	Dynamic mapping of conical intersection seams: A general method for incorporating the geometric phase in adiabatic dynamics in polyatomic systems. Journal of Chemical Physics, 2017, 147, 044109.	3.0	25
59	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.	3.0	25
60	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.	4.6	25
61	Stereodynamical control of product branching in multi-channel barrierless hydrogen abstraction of CH₃OH by F. Chemical Science, 2019, 10, 7994-8001.	7.4	24
62	Energy transfer between vibrationally excited carbon monoxide based on a highly accurate six-dimensional potential energy surface. Journal of Chemical Physics, 2020, 153, 054310.	3.0	24
63	Adiabatic and nonadiabatic energy dissipation during scattering of vibrationally excited CO from Au(111). Physical Review B, 2019, 100, .	3.2	23
64	Potential energy surfaces for high-energy N + O2 collisions. Journal of Chemical Physics, 2021, 154, 084304.	3.0	23
65	Accurate Determination of Tunneling-Affected Rate Coefficients: Theory Assessing Experiment. Journal of Physical Chemistry Letters, 2017, 8, 3392-3397.	4.6	22
66	Advanced solid-state 1H/31P NMR characterization of pyrophosphate-doped calcium phosphate cements for biomedical applications: The structural role of pyrophosphate. Ceramics International, 2019, 45, 20642-20655.	4.8	22
67	Neural Network Based Quasi-diabatic Representation for S₀ and S₁ States of Formaldehyde. Journal of Physical Chemistry A, 2020, 124, 10132-10142.	2.5	21
68	Capture of SO₃isomers in the oxidation of sulfur monoxide with molecular oxygen. Chemical Communications, 2018, 54, 1690-1693.	4.1	19
69	Low temperature rates for key steps of interstellar gas-phase water formation. Science Advances, 2018, 4, eaar3417.	10.3	19
70	A Quasi-Diabatic Representation of the 1,2¹A States of Methylamine. Journal of Physical Chemistry A, 2019, 123, 5231-5241.	2.5	19
71	Unexpected Indirect Dynamics in Base-Induced Elimination. Journal of the American Chemical Society, 2019, 141, 20300-20308.	13.7	19
72	Statistical quantum mechanical approach to diatomâ€“diatom capture dynamics and application to ultracold KRb + KRb reaction. Journal of Chemical Physics, 2020, 152, 241103.	3.0	19

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73	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.	3.0	19
74	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.	4.6	19
75	Photoabsorption Assignments for the Cl$f1B2 â†•Xl$f1A1 Vibronic Transitions of SO2, Using New Ab Initio Potential Energy and Transition Dipole Surfaces. Journal of Physical Chemistry A, 2017, 121, 1012-1021.	2.5	18
76	Combined Experimentalâ€“Theoretical Study of the OH + CO â†' H + CO₂ Reaction Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 1229-1236.	4.6	18
77	The near-UV absorber OSSO and its isomers. Chemical Communications, 2018, 54, 4517-4520.	4.1	18
78	Adsorption of methylene blue and its N-demethylated derivatives on the (111) face of coinage metals: The importance of dispersion interactions. Journal of Chemical Physics, 2017, 146, 164701.	3.0	17
79	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.	4.6	17
80	The Monetite Structure Probed by Advanced Solid-State NMR Experimentation at Fast Magic-Angle Spinning. International Journal of Molecular Sciences, 2019, 20, 6356.	4.1	17
81	A Global Full-Dimensional Potential Energy Surface for the K₂Rb₂ Complex and Its Lifetime. Journal of Physical Chemistry Letters, 2020, 11, 2605-2610.	4.6	17
82	Full-dimensional quantum stereodynamics of the non-adiabatic quenching of OH(A2Î£+) by H2. Nature Chemistry, 2021, 13, 909-915.	13.6	17
83	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.	7.4	16
84	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.	2.5	16
85	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.	3.0	16
86	Fermi resonance controlled product branching in the H + HOD reaction. Physical Chemistry Chemical Physics, 2018, 20, 17029-17037.	2.8	16
87	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.	2.5	16
88	Isomer-specific kinetics of the C ⁺ + H ₂ O reaction at the temperature of interstellar clouds. Science Advances, 2021, 7, .	10.3	16
89	Autodetachment from Vibrationally Excited Vinylidene Anions. Journal of Physical Chemistry Letters, 2018, 9, 1058-1063.	4.6	15
90	Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). Journal of Chemical Physics, 2018, 149, 044703.	3.0	15

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91	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.	3.2	15
92	Dynamical interference in the vibronic bond breaking reaction of HCO. Science Advances, 2019, 5, eaau0582.	10.3	15
93	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.	2.8	15
94	Orbiting resonances in formaldehyde reveal coupling of roaming, radical, and molecular channels. Science, 2021, 374, 1122-1127.	12.6	15
95	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
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.	2.8	14
97	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.	3.1	14
98	Vibrational mode-specificity in the dynamics of the Cl + C2H6 â†' HCl + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 114303.	3.0	14
99	Nonadiabatic photodissociation dynamics of the hydroxymethyl radical via the 22A(3s) Rydberg state: A four-dimensional quantum study. Journal of Chemical Physics, 2017, 146, 224306.	3.0	13
100	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.	2.8	13
101	Au₂⁺ cannot catalyze conversion of methane to ethene at low temperature. Catalysis Science and Technology, 2019, 9, 2767-2780.	4.1	13
102	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.	3.0	13
103	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.	3.0	13
104	The formation and mechanism of nano-monocrystalline Î³-Fe₂O₃ with graphene-shell for high-performance lithium ion batteries. RSC Advances, 2016, 6, 51777-51782.	3.6	12
105	Rotational excitation of the interstellar NH2 radical by H2. Journal of Chemical Physics, 2017, 146, 064309.	3.0	12
106	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.	2.8	12
107	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.	3.1	12
108	Diffraction of CH₄ from a Metal Surface. Journal of Physical Chemistry Letters, 2019, 10, 1574-1580.	4.6	12

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109	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.	3.1	12
110	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.	5.3	12
111	Acetylene hydrogenation catalyzed by bare and Ni doped CeO₂(110): the role of frustrated Lewis pairs. Physical Chemistry Chemical Physics, 2022, 24, 11295-11304.	2.8	12
112	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.	3.0	11
113	Solid-State NMR Rationalizes the Bone-Adhesive Properties of Serine- and Phosphoserine-Bearing Calcium Phosphate Cements by Unveiling Their Organic/Inorganic Interface. Journal of Physical Chemistry C, 2020, 124, 21512-21531.	3.1	11
114	Full-Dimensional Potential Energy Surface for Ro-vibrationally Inelastic Scattering between H₂ Molecules. Journal of Chemical Theory and Computation, 2021, 17, 6747-6756.	5.3	11
115	Stereodynamical Control of Cold Collisions of Polyatomic Molecules with Atoms. Journal of Physical Chemistry Letters, 2022, 13, 1777-1784.	4.6	11
116	Globally Accurate Full-Dimensional Potential Energy Surface for H₂ + HCl Inelastic Scattering. Journal of Physical Chemistry A, 2019, 123, 6578-6586.	2.5	10
117	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.	2.8	10
118	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.	7.1	10
119	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.	4.6	10
120	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.	3.1	10
121	Full-dimensional quantum studies of vibrational energy transfer dynamics between H₂O and Ar: theory assessing experiment. Physical Chemistry Chemical Physics, 2022, 24, 13542-13549.	2.8	10
122	Final State Resolved Quantum Predissociation Dynamics of SO₂(Cl¹B₂) and Its Isotopomers via a Crossing with a Singlet Repulsive State. Journal of Physical Chemistry A, 2017, 121, 4930-4938.	2.5	9
123	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
124	First-principles dynamics of collisional intersystem crossing: resonance enhanced quenching of C(¹D) by N₂. Physical Chemistry Chemical Physics, 2019, 21, 8645-8653.	2.8	9
125	Bond dissociation energy of Au2+: A guided ion beam and theoretical investigation. Journal of Chemical Physics, 2019, 150, 174305.	3.0	9
126	Quasiclassical simulations based on cluster models reveal vibration-facilitated roaming in the isomerization of CO adsorbed on NaCl. Nature Chemistry, 2021, 13, 249-254.	13.6	9

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127	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.	4.6	9
128	Quantum Stereodynamics of H₂ Scattering from Co(0001): Influence of Reaction Channels. Journal of Physical Chemistry C, 2019, 123, 16223-16231.	3.1	8
129	Photoelectronâ€“Photofragment Coincidence Studies on the Dissociation Dynamics of the OHâ€“CH₄ Complex. Journal of Physical Chemistry A, 2019, 123, 4825-4833.	2.5	8
130	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.	3.1	8
131	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.	2.5	8
132	Quantitative phase analyses of biomedical pyrophosphate-bearing monetite and brushite cements by solid-state NMR and powder XRD. Ceramics International, 2020, 46, 11000-11012.	4.8	8
133	A Time-Independent Quantum Approach to Ro-vibrationally Inelastic Scattering between Atoms and Triatomic Molecules. Journal of Physical Chemistry A, 2021, 125, 6864-6871.	2.5	8
134	Excess lithium storage in LiFePO₄-Carbon interface by ball-milling. Functional Materials Letters, 2016, 09, 1650053.	1.2	7
135	Temperature and Pressure Dependences of the Reactions of Fe⁺ with Methyl Halides CH₃X (X = Cl, Br, I): Experiments and Kinetic Modeling Results. Journal of Physical Chemistry A, 2017, 121, 4058-4068.	2.5	7
136	First-principles C band absorption spectra of SO₂ and its isotopologues. Journal of Chemical Physics, 2017, 146, 154305.	3.0	7
137	Charge Transfer Doping Induced Conformational Ordering of a Non-Crystalline Conjugated Polymer. Journal of Physical Chemistry C, 2017, 121, 23817-23826.	3.1	7
138	Surprising behaviors in the temperature dependent kinetics of diatomic interhalogens with anions and cations. Journal of Chemical Physics, 2017, 146, 214307.	3.0	7
139	Machine Learning. Journal of Physical Chemistry A, 2018, 122, 879-879.	2.5	7
140	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.	2.8	7
141	Scattering Dynamics of Glycine, H2O, and CO2 on Highly Oriented Pyrolytic Graphite. Journal of Physical Chemistry C, 2019, 123, 3605-3621.	3.1	7
142	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.	2.5	7
143	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.	2.0	7
144	Rotational Modulation of Ãƒ2Aâ€³-State Photodissociation of HCO via Rennerâ€“Teller Nonadiabatic Transitions. Journal of Physical Chemistry Letters, 2021, 12, 6582-6588.	4.6	7

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145	Semiclassical Trajectory Studies of Reactive and Nonreactive Scattering of OH(A²Î£⁺) by H₂ Based on an Improved Fullâ€Dimensional Ab Initio Diabatic Potential Energy Matrix. ChemPhysChem, 2022, 23, .	2.1	7
146	Experimental and theoretical studies of the reactions of ground-state sulfur atoms with hydrogen and deuterium. Journal of Chemical Physics, 2017, 147, 134302.	3.0	6
147	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.	2.5	6
148	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.	5.3	6
149	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.	3.0	5
150	Trapping of different stages of BaTiO₃reduction with LiH. RSC Advances, 2020, 10, 35356-35365.	3.6	5
151	Insights into the Formation of Hydroxyl Radicals with Nonthermal Vibrational Excitation in the Meinel Airglow. Journal of Physical Chemistry Letters, 2021, 12, 1822-1828.	4.6	5
152	Insights into adsorption, diffusion, and reactions of atomic nitrogen on a highly oriented pyrolytic graphite surface. Journal of Chemical Physics, 2021, 154, 074708.	3.0	5
153	Reactive and Nonreactive Collisions between NO(X²Î) and O(³P) under Hyperthermal Conditions. Journal of Physical Chemistry A, 2022, 126, 4277-4285.	2.5	5
154	Frustrated Lewis Pairs in Heterogeneous Catalysis: Theoretical Insights. Molecules, 2022, 27, 3734.	3.8	5
155	Quantum dynamics of ClH2Oâ¯ photodetachment: Isotope effect and impact of anion vibrational excitation. Journal of Chemical Physics, 2018, 148, 064305.	3.0	4
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