Daiqian Xie

List of Publications by Year in descending order

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222 papers	5,469 citations	70961 41 h-index	133063 59 g-index
227 all docs	227 docs citations	227 times ranked	3799 citing authors

#	Article	IF	Citations
1	Observation of Feshbach Resonances in the F + H2 -> HF + H Reaction. Science, 2006, 311, 1440-1443.	6.0	278
2	Quantum dynamics of polyatomic dissociative chemisorption on transition metal surfaces: mode specificity and bond selectivity. Chemical Society Reviews, 2016, 45, 3621-3640.	18.7	140
3	Nonadiabatic Tunneling in Photodissociation of Phenol. Journal of the American Chemical Society, 2016, 138, 7828-7831.	6.6	126
4	Mode selectivity in methane dissociative chemisorption on Ni(111). Chemical Science, 2013, 4, 3249.	3.7	115
5	A new ab initio potential-energy surface of HO2(X2Aâ€³) and quantum studies of HO2 vibrational spectrum and rate constants for the H+O2â†”O+OH reactions. Journal of Chemical Physics, 2005, 122, 244305.	1.2	106
6	Communication: A chemically accurate global potential energy surface for the HO + CO â†’ H + CO2 reaction. Journal of Chemical Physics, 2012, 136, 041103.	1.2	102
7	Enhancing dissociative chemisorption of H ₂ O on Cu(111) via vibrational excitation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 10224-10227.	3.3	89
8	Vibronic origin of sulfur mass-independent isotope effect in photoexcitation of SO ₂ and the implications to the early earthâ€™s atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17697-17702.	3.3	88
9	High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH₂OO). Journal of Physical Chemistry Letters, 2014, 5, 2364-2369.	2.1	86
10	Cobalt/zinc dual-sites coordinated with nitrogen in nanofibers enabling efficient and durable oxygen reduction reaction in acidic fuel cells. Journal of Materials Chemistry A, 2020, 8, 3686-3691.	5.2	76
11	A permutationally invariant full-dimensional ab initio potential energy surface for the abstraction and exchange channels of the H + CH4 system. Journal of Chemical Physics, 2015, 142, 204302.	1.2	71
12	A novel phosphotungstic acid-supported single metal atom catalyst with high activity and selectivity for the synthesis of NH₃ from electrochemical N₂ reduction: a DFT prediction. Journal of Materials Chemistry A, 2019, 7, 19838-19845.	5.2	69
13	Mechanistic Insights into a Classic Wonder Drugâ€”Aspirin. Journal of the American Chemical Society, 2015, 137, 70-73.	6.6	66
14	Pathways for methanol steam reforming involving adsorbed formaldehyde and hydroxyl intermediates on Cu(111): density functional theory studies. Physical Chemistry Chemical Physics, 2011, 13, 9622.	1.3	61
15	Accurate quantum mechanical calculations of differential and integral cross sections and rate constant for the O+OH reaction using an ab initio potential energy surface. Journal of Chemical Physics, 2008, 128, 014303.	1.2	60
16	Pathways of Methanol Steam Reforming on PdZn and Comparison with Cu. Journal of Physical Chemistry C, 2011, 115, 20583-20589.	1.5	60
17	Vibrationally mediated bond selective dissociative chemisorption of HOD on Cu(111). Chemical Science, 2013, 4, 503-508.	3.7	60
18	Initial steps in methanol steam reforming on PdZn and ZnO surfaces: Density functional theory studies. Surface Science, 2011, 605, 750-759.	0.8	58

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19	Three-Dimensional Photodissociation Dynamics of Rotational State Selected Methyl Iodide. Journal of Physical Chemistry A, 2000, 104, 1009-1019.	1.1	57
20	Effects of reactant internal excitation and orientation on dissociative chemisorption of H2O on Cu(111): Quasi-seven-dimensional quantum dynamics on a refined potential energy surface. Journal of Chemical Physics, 2013, 138, 044704.	1.2	57
21	Rate constant for OH(Î2)+O(P3)â†'H(S2)+O2(Î£gâ^'3) reaction on an improved ab initio potential energy surface and implications for the interstellar oxygen problem. Journal of Chemical Physics, 2007, 127, 024304.	1.2	56
22	State-to-state photodissociation dynamics of triatomic molecules: H2O in the B band. Journal of Chemical Physics, 2012, 136, 034302.	1.2	56
23	Controlling the self-assembly pathways of amphiphilic block copolymers into vesicles. Soft Matter, 2012, 8, 7865.	1.2	56
24	Ab initio potential energy surface and rovibrational spectra of Heâ€"CO2. Journal of Chemical Physics, 1998, 109, 10284-10292.	1.2	53
25	Precision test of statistical dynamics with state-to-state ultracold chemistry. Nature, 2021, 593, 379-384.	13.7	53
26	State-to-State Dynamics of H + O2 Reaction, Evidence for Nonstatistical Behavior. Journal of the American Chemical Society, 2008, 130, 14962-14963.	6.6	52
27	First-principles study of decomposition of NH3 on Ir(100). Surface Science, 2008, 602, 1288-1294.	0.8	50
28	Fully Coriolis-Coupled Quantum Studies of the H + O₂ (Ï…_i = 0â^'2,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Cross Sections and Rate Constants. Journal of Physical Chemistry A, 2008, 112, 602-611.	1.1	50
29	Full-Dimensional Quantum State-to-State Nonadiabatic Dynamics for Photodissociation of Ammonia in its A-Band. Journal of Physical Chemistry Letters, 2014, 5, 1055-1060.	2.1	50
30	Methyl Formate Pathway in Methanol Steam Reforming on Copper: Density Functional Calculations. ACS Catalysis, 2011, 1, 1263-1271.	5.5	47
31	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
32	Advances and New Challenges to Bimolecular Reaction Dynamics Theory. Journal of Physical Chemistry Letters, 2020, 11, 8844-8860.	2.1	46
33	Global analytical potential energy surfaces for HO2(XÌƒAâ€³2) based on high-levelab initiocalculations. Journal of Chemical Physics, 2007, 126, 074315.	1.2	45
34	Differential and Integral Cross Sections for the H + O2â†' OH + O Combustion Reaction. Journal of Physical Chemistry A, 2007, 111, 5349-5352.	1.1	44
35	A new potential energy surface and predicted infrared spectra of Heâ€"CO2: Dependence on the antisymmetric stretch of CO2. Journal of Chemical Physics, 2008, 128, 124323.	1.2	44
36	Ab initio determination of potential energy surfaces for the first two UV absorption bands of SO2. Journal of Chemical Physics, 2013, 139, 014305.	1.2	43

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37	Density functional theory studies on molecular structure and IR spectra of 9-methyladenine: A scaled quantum mechanical force field approach. International Journal of Quantum Chemistry, 2000, 76, 686-699.	1.0	42
38	Comparison of Chebyshev, Faber, and Lanczos propagation-based methods for calculating resonances. Journal of Chemical Physics, 2000, 112, 5263-5269.	1.2	42
39	Quantum Dynamics of the H + O2â† ' O + OH Reaction on an Accurate ab Initio Potential Energy Surface. Journal of Physical Chemistry B, 2006, 110, 23641-23643.	1.2	42
40	Supermolecule density functional calculations suggest a key role for solvent in alkaline hydrolysis of p-nitrophenyl phosphate. Chemical Communications, 2007, , 1638.	2.2	42
41	A new potential energy surface and predicted infrared spectra of the Arâ€"CO2 van der Waals complex. Journal of Chemical Physics, 2009, 130, 224311.	1.2	42
42	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
43	Nature of Photoinduced Quenching Traps in Methylammonium Lead Triiodide Perovskite Revealed by Reversible Photoluminescence Decline. ACS Photonics, 2018, 5, 2034-2043.	3.2	42
44	Analysis of the HO2Vibrational Spectrum on an Accurate Ab Initio Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2007, 111, 10353-10361.	1.1	39
45	Five-dimensional ab initio potential energy surface and predicted infrared spectra of H2â€"CO2 van der Waals complexes. Journal of Chemical Physics, 2007, 126, 204304.	1.2	37
46	State-to-State Photodissociation Dynamics of H₂O in the B-band: Competition between Two Coexisting Nonadiabatic Pathways. Journal of Physical Chemistry A, 2013, 117, 6940-6947.	1.1	37
47	Hydroxyl super rotors from vacuum ultraviolet photodissociation of water. Nature Communications, 2019, 10, 1250.	5.8	37
48	CALCULATION OF TRANSITION AMPLITUDES WITH A SINGLE LANCZOS PROPAGATION. Journal of Theoretical and Computational Chemistry, 2002, 01, 173-185.	1.8	36
49	Potential energy surfaces and predicted infrared spectra for van der Waals complexes: dependence on one intramolecular vibrational coordinate. International Reviews in Physical Chemistry, 2007, 26, 487-520.	0.9	36
50	Theoretical studies of <mml:math altimg="si7.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/common/struct-bib/dtd" xmlns:ce="http://www.elsev. Chemical Rate Coefficients of the HCl + OH â† ' Cl + H₂O Reaction from Ring Polymer Molecular Dynamics. Journal of Physical Chemistry A, 2016, 120, 3433-3440.	1.2	36
51		1.1	36
52	Low temperature rate constants for the N(4S) + CH(X2Îr) reaction. Implications for N2 formation cycles in dense interstellar clouds. Physical Chemistry Chemical Physics, 2013, 15, 13888.	1.3	34
53	Communication: Rigorous quantum dynamics of O + O2 exchange reactions on an ab initio potential energy surface substantiate the negative temperature dependence of rate coefficients. Journal of Chemical Physics, 2014, 141, 081102.	1.2	34
54	Site-specific dissociation dynamics of H2/D2 on Ag(111) and Co(0001) and the validity of the site-averaging model. Journal of Chemical Physics, 2015, 143, 114706.	1.2	34

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55	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
56	Electronic excitations of green fluorescent proteins: Protonation states of chromophore model compound in solutions. Journal of Computational Chemistry, 2005, 26, 1487-1496.	1.5	32
57	State-to-state quantum dynamics of the O(P3)+OH(Î2)â†’H(S2)+O2(Î£3gâ^') reaction. Journal of Chemical Physics, 2010, 133, 054302.	1.2	32
	Ab Initio Potential Energy Surfaces for Both the Ground (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 642 Td (xmlns:mml="		
58			

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73	A theoretical study of solvent effects on tautomerism and electronic absorption spectra of 3-hydroxy-2-mercaptopyridine and 2,3-dihydroxypyridine. Journal of Computational Chemistry, 2004, 25, 1833-1839.	1.5	27
74	A three-dimensional ab initio potential energy surface and predicted infrared spectra for the Heâ€“N2O complex. Journal of Chemical Physics, 2006, 124, 144317.	1.2	27
75	Stateâ€toâ€state photodissociation dynamics of the water molecule. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1350.	6.2	27
76	Theoretical study of predissociation dynamics of HCN/DCN in their first absorption bands. Journal of Chemical Physics, 2002, 116, 10626-10635.	1.2	26
77	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
78	Intermolecular potential energy surface, microwave and infrared spectra of the Krâ€“CO2 complex from ab initio calculations. Chemical Physics Letters, 2011, 511, 229-234.	1.2	24
79	Communication: State-to-state differential cross sections for H2O($ilde B$Bìf) photodissociation. Journal of Chemical Physics, 2011, 134, 231103.	1.2	23
80	Signatures of non-adiabatic dynamics in the fine-structure state distributions of the OH(Xìf/Aìf) products in the B-band photodissociation of H2O. Journal of Chemical Physics, 2015, 142, 124317.	1.2	23
81	Six-dimensional quantum dynamics of dissociative chemisorption of H2 on Co(0001) on an accurate global potential energy surface. Physical Chemistry Chemical Physics, 2015, 17, 23346-23355.	1.3	23
82	An interaction-asymptotic region decomposition method for general state-to-state reactive scatterings. Journal of Chemical Physics, 2019, 150, 134105.	1.2	23
83	Hydrogen bonding and solvatochromatic shift of the lowest1(n, ?*) excitation of s-tetrazine in its hydrated clusters and dilute solutions. Journal of Computational Chemistry, 2004, 25, 1487-1495.	1.5	22
84	Product fine-structure resolved photodissociation dynamics: The A band of H2O. Journal of Chemical Physics, 2014, 140, 024310.	1.2	22
85	Accurate Determination of Tunneling-Affected Rate Coefficients: Theory Assessing Experiment. Journal of Physical Chemistry Letters, 2017, 8, 3392-3397.	2.1	22
86	Quantum calculations of highly excited vibrational spectrum of sulfur dioxide. III. Emission spectra from the Cìfâ€Š1B2 state. Journal of Chemical Physics, 1999, 111, 7782-7788.	1.2	21
87	An ab initio potential energy surface and predissociative resonances of HArF. Journal of Chemical Physics, 2004, 120, 4273-4280.	1.2	21
88	Electronic Excitations of Green Fluorescent Proteins:â€‰ Modeling Solvatochromatic Shifts of Red Fluorescent Protein Chromophore Model Compound in Aqueous Solutions. Journal of Physical Chemistry B, 2007, 111, 14055-14063.	1.2	21
89	Nanoparticle encapsulation in vesicles formed by amphiphilic diblock copolymers. Soft Matter, 2017, 13, 7840-7847.	1.2	21
90	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in Solution. Journal of Chemical Theory and Computation, 2018, 14, 5787-5796.	2.3	21

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91	Identification of the Band Gap Energy of Two-dimensional (OA)₂(MA)_{nâ^'1}Pb_nI_{3n+1} Perovskite with up to 10 Layers. Journal of Physical Chemistry Letters, 2019, 10, 7025-7030.	2.1	21
92	Direct calculation of cumulative reaction probabilities from Chebyshev correlation functions. Journal of Chemical Physics, 2002, 116, 6391-6396.	1.2	20
93	A refined potential energy function for the electronic ground state of NO₂. Molecular Physics, 1996, 88, 1349-1355.	0.8	19
94	Theoretical studies for structures and energetics of Rgn?N2O (Rg?He, Ne, Ar) clusters. Journal of Computational Chemistry, 2003, 24, 1839-1845.	1.5	19
95	A five-dimensional potential energy surface and predicted infrared spectra for the N2O-hydrogen complexes. Journal of Chemical Physics, 2006, 125, 174310.	1.2	19
96	A global coupled cluster potential energy surface for HCl + OH â†" Cl + H₂O. Physical Chemistry Chemical Physics, 2017, 19, 9770-9777.	1.3	19
97	A full-dimensional potential energy surface and quantum dynamics of inelastic collision process for H2â€"HF. Journal of Chemical Physics, 2018, 148, 184301.	1.2	19
98	A new full-dimensional ab initio intermolecular potential energy surface and vibrational states for (HF)2 and (DF)2. Journal of Chemical Physics, 2019, 150, 154302.	1.2	19
99	Water Photolysis and Its Contributions to the Hydroxyl Dayglow Emissions in the Atmospheres of Earth and Mars. Journal of Physical Chemistry Letters, 2020, 11, 9086-9092.	2.1	19
100	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
101	Mechanistic insights into the H+O2â†'OH+O reaction from quasi-classical trajectory studies on a new ab initio potential energy surface. Chemical Physics, 2008, 349, 181-187.	0.9	18
102	Effects of reactant rotational excitation on H + O2â†' OH + O reaction rate constant: quantum wave packet, quasi-classical trajectory and phase space theory calculations. Physical Chemistry Chemical Physics, 2009, 11, 4715.	1.3	18
103	An improved coupled-states approximation including the nearest neighbor Coriolis couplings for diatom-diatom inelastic collision. Journal of Chemical Physics, 2018, 148, 084101.	1.2	18
104	Ab initio potential energy surface and rovibrational spectra of Neâ€"N2O. Chemical Physics Letters, 2002, 351, 149-157.	1.2	17
105	Ab initio intermolecular potential-energy surface and microwave spectra for the Neâ€"OCS complex. Journal of Chemical Physics, 2005, 122, 234312.	1.2	17
106	Ab initio potential energy surface and predicted microwave spectra for Arï£¿OCS dimer and structures of Arnï£¿OCS (n = 2â€"14) clusters. Journal of Computational Chemistry, 2006, 27, 1045-1053.	1.5	17
107	Path integral Monte Carlo study of CO2 solvation in He4 clusters. Journal of Chemical Physics, 2008, 128, 224513.	1.2	17
108	An experimental and theoretical investigation of the N(⁴S) + C₂(¹Î£_g⁺) reaction at low temperature. Physical Chemistry Chemical Physics, 2014, 16, 14212-14219.	1.3	17

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109	Three-Dimensional Diabatic Potential Energy Surfaces for the Photodissociation of Thiophenol. Journal of Physical Chemistry A, 2017, 121, 8432-8439.	1.1	17
110	Breakdown of energy transfer gap laws revealed by full-dimensional quantum scattering between HF molecules. Nature Communications, 2019, 10, 4658.	5.8	17
111	Electronically Excited OH Super-rotors from Water Photodissociation by Using Vacuum Ultraviolet Free-Electron Laser Pulses. Journal of Physical Chemistry Letters, 2020, 11, 7617-7623.	2.1	17
112	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
113	Theoretical Study of the aza-Wittig Reactions of X3PNH (X=H and Cl) with Formaldehyde in Gas Phase and in Solution. Journal of Physical Chemistry A, 2002, 106, 9053-9058.	1.1	16
114	Medium effects on the lowest 1(n,Ï€*) excitation of 1,2,3-triazine in water. Chemical Physics Letters, 2003, 368, 377-383.	1.2	16
115	Density functional study of the adsorption of Na and K on Rh(111). Surface Science, 2004, 553, 13-22.	0.8	16
116	Nonadiabatic Dynamics of Ãƒ-State Photodissociation of Ammonia: A Four-Dimensional Wave Packet Study. Journal of Physical Chemistry A, 2010, 114, 3121-3126.	1.1	16
117	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
118	Superfluid response of 4HeNâ€“N2O clusters probed by path integral Monte Carlo simulations. Journal of Molecular Spectroscopy, 2011, 267, 136-143.	0.4	15
119	Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). Journal of Chemical Physics, 2018, 149, 044703.	1.2	15
120	Aqueous Self-Assembly of Amphiphilic Cyclic Brush Block Copolymers as Asymmetry-Tunable Building Blocks. Macromolecules, 2019, 52, 7042-7051.	2.2	15
121	Dynamical interference in the vibronic bond breaking reaction of HCO. Science Advances, 2019, 5, eaau0582.	4.7	15
122	Three body photodissociation of the water molecule and its implications for prebiotic oxygen production. Nature Communications, 2021, 12, 2476.	5.8	15
123	Vibrationally excited molecular hydrogen production from the water photochemistry. Nature Communications, 2021, 12, 6303.	5.8	15
124	Theoretical studies of force fields and IR spectra of isocytosine. International Journal of Quantum Chemistry, 1999, 72, 53-60.	1.0	14
125	Reactivity of Metaphosphate and Thiometaphosphate in Water:â€‰ A DFT Study. Journal of Physical Chemistry A, 2005, 109, 11295-11303.	1.1	14
126	State to state photodissociation dynamics of D2O in the B band. Journal of Chemical Physics, 2013, 139, 114303.	1.2	14

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127	Precisely Controlled Incorporation of Drug Nanoparticles in Polymer Vesicles by Amphiphilic Copolymer Tethers. Macromolecules, 2018, 51, 6810-6817.	2.2	14
128	Rovibrational bound states of the Neâ€“OCS complex. Chemical Physics Letters, 1998, 287, 162-168.	1.2	13
129	Initial Decomposition of Methanol and Water on In₂O₃(110): A Periodic DFT Study. Chinese Journal of Chemistry, 2012, 30, 2036-2040.	2.6	13
130	Ab initio potential energy surface and rovibrational spectrum of Arâ˜HCCCN. Journal of Chemical Physics, 2004, 121, 2630.	1.2	12
131	Three-dimensional ab initio potential-energy surface and rovibrational spectra of the H2â€“Kr complex. Journal of Chemical Physics, 2005, 123, 134323.	1.2	12
132	Quantum dynamics of vibrationâ€“vibration energy transfer for vibrationally excited HF colliding with H₂. Journal of Computational Chemistry, 2019, 40, 1084-1090.	1.5	12
133	Ab initio potential energy surface and excited vibrational states for the electronic ground state of Li2H. Science in China Series B: Chemistry, 1997, 40, 342-347.	0.8	11
134	A DFT investigation of potential energy surface and vibrational properties of hydrogen adsorbed on the Rh(111) surface. Surface Science, 2004, 550, 15-20.	0.8	11
135	Theoretical Study of General Base-Catalyzed Hydrolysis of Aryl Esters and Implications for Enzymatic Reactions. Journal of Physical Chemistry B, 2005, 109, 5259-5266.	1.2	11
136	New ab initio coupled potential energy surfaces for the Br(2P3/2, 2P1/2) + H2 reaction. Journal of Chemical Physics, 2011, 135, 164311.	1.2	11
137	Theoretical Study of the State-to-State Photodissociation Dynamics of the Vibrationally Excited Water Molecule in the B Band. Journal of Physical Chemistry A, 2014, 118, 9220-9227.	1.1	11
138	Quantum wavepacket method for state-to-state reactive cross sections in hyperspherical coordinates. Journal of Chemical Physics, 2018, 149, 174103.	1.2	11
139	Nonadiabatic Effect in Photodissociation Dynamics of Thiophenol via the ¹Ï€Ï€* State. Journal of Physical Chemistry A, 2018, 122, 5375-5382.	1.1	11
140	Stereodynamical Control of Cold Collisions of Polyatomic Molecules with Atoms. Journal of Physical Chemistry Letters, 2022, 13, 1777-1784.	2.1	11
141	Ab initio studies for the photodissociation mechanism of hydroxyacetone. Journal of Computational Chemistry, 2003, 24, 931-938.	1.5	10
142	First-Principles Study of K and Cs Adsorbed on Pd(111). Journal of Physical Chemistry B, 2006, 110, 23904-23910.	1.2	10
143	Theoretical studies on the potential energy surfaces and vibrational energy levels of HXeF and HXeCl. Science in China Series B: Chemistry, 2007, 50, 7-10.	0.8	10
144	Theoretical prediction of the noble gas complexes HeAuF and NeAuF. Science in China Series B: Chemistry, 2009, 52, 1987-1990.	0.8	10

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145	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
146	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
147	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
148	Mechanisms of Oxygen Passivation on Surface Defects in MAPbI₃ Revealed by First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 3731-3737.	1.5	10
149	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
150	Ab initio potential energy surface of Neî—¸OCS. Chemical Physics Letters, 1997, 275, 494-498.	1.2	9
151	A computational study on the mechanism for the GaCl3-catalyzed [4+1] cycloaddition of Î±,Î²-unsaturated ketone and 2,6-dimethylphenyl isocyanide. Tetrahedron, 2005, 61, 507-512.	1.0	9
152	Full-Dimensional Quantum Dynamics of Vibrational Mediated Photodissociation of HOD in Its B Band. Journal of Physical Chemistry A, 2015, 119, 12062-12072.	1.1	9
153	Dynamics of carbon monoxide dissociation on Co(112Ì„0). Physical Chemistry Chemical Physics, 2017, 19, 12826-12837.	1.3	9
154	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
155	A Full-Dimensional ab initio Intermolecular Potential Energy Surface and Dipole Moment Surfaces for H2O-Ar. Current Chinese Science, 2022, 2, 325-334.	0.2	9
156	Predissociation of HCN/DCN in Two Lowest-Lying Singlet Excited States:â€‰ Effect of Fermi Resonances on Spectra and Dynamics. Journal of Physical Chemistry A, 2002, 106, 10174-10183.	1.1	8
157	State-to-state quantum dynamics of the O(3P) + NH(X3Î£â^) reaction on the three lowest-lying electronic states of HNO/HON. Journal of Chemical Physics, 2013, 138, 024308.	1.2	8
158	A full-dimensional ab initio potential energy surface and rovibrational energies of the Arâ€“HF complex. Molecular Physics, 2018, 116, 835-842.	0.8	8
159	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
160	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
161	ELECTRONIC EXCITATIONS OF GREEN FLUORESCENT PROTEINS: MODELING SOLVATOCHROMATIC SHIFTS OF CHROMOPHORE MODEL COMPOUNDS IN SOLUTIONS. Journal of Theoretical and Computational Chemistry, 2006, 05, 375-390.	1.8	7
162	Theoretical Investigation on the GaCl₃-Catalyzed Ring-Closing Metathesis Reaction of N-2,3-Butadienyl-2-propynyl-1-amine:â€‰ Three-Membered Ring versus Four-Membered Ring Mechanism. Journal of Physical Chemistry A, 2007, 111, 9387-9392.	1.1	7

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163	VIBRATIONALLY AVERAGED POTENTIAL ENERGY SURFACES AND PREDICTED INFRARED SPECTRA OF THE Heâ€“18O13C18O AND Heâ€“16O13C16O COMPLEXES. Journal of Theoretical and Computational Chemistry, 2008, 07, 707-717.	1.8	7
164	Interaction specific binding hotspots in Endonuclease colicin-immunity protein complex from MD simulations. Science China Chemistry, 2013, 56, 1143-1151.	4.2	7
165	State-to-state quantum dynamics of the N(4S) + CH(Xâ€‰2Î) â†' CN(Xâ€‰2Î£+,A2Î) + H(2S) reactions. Journal of Chemical Physics, 2013, 139, 124313.	1.2	7
166	Predicted infrared spectra in the HF stretching band of the H2â€“HF complex. Journal of Chemical Physics, 2018, 149, 094307.	1.2	7
167	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
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