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	Dissection of the Multichannel Reaction O(3P) + C2H2: Differential Cross-Sections and Product Energy Distributions. Molecules, 2022, 27, 754.	1.7	2
2	Adiabatic potential energy surfaces and photodissociation mechanisms for highly excited states of H2O. Chinese Journal of Chemical Physics, 2022, 35, 104-116.	0.6	7
3	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
4	Stereodynamical Control of Cold Collisions of Polyatomic Molecules with Atoms. Journal of Physical Chemistry Letters, 2022, 13, 1777-1784.	2.1	11
5	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
6	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
7	Mechanisms and Kinetics Studies of Butylated Hydroxytoluene Degradation to Isobutene. Journal of Physical Chemistry A, 2022, , .	1.1	2
8	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
9	Interaction-Asymptotic Region Decomposition Method for an Insertion Reaction: Application to the S(¹D) + H₂ Reaction. Journal of Physical Chemistry A, 2021, 125, 2007-2018.	1.1	5
10	Quantum dynamics of the energy transfer for vibrationally excited HF (v = 7) colliding with D2 (v = 0): Theory assessing experiment. Journal of Chemical Physics, 2021, 154, 114303.	1.2	3
11	Interaction-Asymptotic Region Decomposition Method for a Triatomic Reactive Scattering with Symmetry Adoption. Journal of Physical Chemistry A, 2021, 125, 2460-2471.	1.1	4
12	Three body photodissociation of the water molecule and its implications for prebiotic oxygen production. Nature Communications, 2021, 12, 2476.	5.8	15
13	Precision test of statistical dynamics with state-to-state ultracold chemistry. Nature, 2021, 593, 379-384.	13.7	53
14	Strong isotope effect in the VUV photodissociation of HOD: A possible origin of D/H isotope heterogeneity in the solar nebula. Science Advances, 2021, 7, .	4.7	5
15	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
16	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
17	Spontaneous Polarity Flipping in a 2D Heterobilayer Induced by Fluctuating Interfacial Carrier Flows. Nano Letters, 2021, 21, 6773-6780.	4.5	7
18	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

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19	A full-dimensional ab initio intermolecular potential energy surface and rovibrational spectra for OCâ€“HF and OCâ€“DF. Journal of Chemical Physics, 2021, 155, 084302.	1.2	2
20	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
21	Quantum Dynamics of Rotational Energy Transfer Processes for N₂â€“HF and N₂â€“DF Systems. Journal of Physical Chemistry A, 2021, 125, 349-355.	1.1	1
22	Vibrationally excited molecular hydrogen production from the water photochemistry. Nature Communications, 2021, 12, 6303.	5.8	15
23	Computational determination of binding modes of 2-acetoxyphenylhept-2-ynyl sulfide to cyclooxygenase-2. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3648-3658.	2.0	2
24	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
25	State-to-state chemical kinetic mechanism for HF chemical lasers. Combustion Theory and Modelling, 2020, 24, 129-141.	1.0	3
26	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
27	Probing the Potential Energy Surfaces of BrCN^{â€“} by Dissociative Electron Attachment. Journal of Physical Chemistry Letters, 2020, 11, 9110-9116.	2.1	5
28	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
29	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
30	Advances and New Challenges to Bimolecular Reaction Dynamics Theory. Journal of Physical Chemistry Letters, 2020, 11, 8844-8860.	2.1	46
31	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
32	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
33	A theoretical study on quantum dynamics of energy transfer for HF colliding with D2. European Physical Journal D, 2020, 74, 1.	0.6	3
34	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
35	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
36	A full-dimensional ab initio intermolecular potential energy surface and ro-vibrational spectra for N2â€“HF and N2â€“DF. Journal of Chemical Physics, 2020, 152, 084304.	1.2	3

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37	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
38	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
39	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
40	Dynamics Studies of O₂ Collision on Pt(111) Using a Global Potential Energy Surface. Journal of Physical Chemistry C, 2020, 124, 10573-10583.	1.5	7
41	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
42	Breakdown of energy transfer gap laws revealed by full-dimensional quantum scattering between HF molecules. Nature Communications, 2019, 10, 4658.	5.8	17
43	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
44	Aqueous Self-Assembly of Amphiphilic Cyclic Brush Block Copolymers as Asymmetry-Tunable Building Blocks. Macromolecules, 2019, 52, 7042-7051.	2.2	15
45	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
46	Molecular insight into chymotrypsin inhibitor 2 resisting proteolytic degradation. Physical Chemistry Chemical Physics, 2019, 21, 5049-5058.	1.3	6
47	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
48	Linking inhibitor motions to proteolytic stability of sunflower trypsin inhibitor-1. RSC Advances, 2019, 9, 13776-13786.	1.7	3
49	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
50	Anomalous kinetics of the reaction between OH and HO₂on an accurate triplet state potential energy surface. Physical Chemistry Chemical Physics, 2019, 21, 12667-12675.	1.3	30
51	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
52	Hydroxyl super rotors from vacuum ultraviolet photodissociation of water. Nature Communications, 2019, 10, 1250.	5.8	37
53	An interaction-asymptotic region decomposition method for general state-to-state reactive scatterings. Journal of Chemical Physics, 2019, 150, 134105.	1.2	23
54	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

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55	Dynamical interference in the vibronic bond breaking reaction of HCO. Science Advances, 2019, 5, eaau0582.	4.7	15
56	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
57	Quantum dynamics of ClH2Oâ¯ photodetachment: Isotope effect and impact of anion vibrational excitation. Journal of Chemical Physics, 2018, 148, 064305.	1.2	4
58	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
59	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
60	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
61	Nature of Photoinduced Quenching Traps in Methylammonium Lead Triiodide Perovskite Revealed by Reversible Photoluminescence Decline. ACS Photonics, 2018, 5, 2034-2043.	3.2	42
62	Stateâ€toâ€state photodissociation dynamics of the water molecule. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1350.	6.2	27
63	Cover Image, Volume 8, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1362.	6.2	1
64	Predicted infrared spectra in the HF stretching band of the H2â€“HF complex. Journal of Chemical Physics, 2018, 149, 094307.	1.2	7
65	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
66	Quantum wavepacket method for state-to-state reactive cross sections in hyperspherical coordinates. Journal of Chemical Physics, 2018, 149, 174103.	1.2	11
67	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
68	Nonadiabatic Effect in Photodissociation Dynamics of Thiophenol via the ¹Ï€Ï€* State. Journal of Physical Chemistry A, 2018, 122, 5375-5382.	1.1	11
69	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
70	Precisely Controlled Incorporation of Drug Nanoparticles in Polymer Vesicles by Amphiphilic Copolymer Tethers. Macromolecules, 2018, 51, 6810-6817.	2.2	14
71	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
72	Vibrational enhancement in the dynamics of ammonia dissociative chemisorption on Ru(0001). Journal of Chemical Physics, 2018, 149, 044703.	1.2	15

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73	Dynamics of carbon monoxide dissociation on Co(112Ì„0). Physical Chemistry Chemical Physics, 2017, 19, 12826-12837.	1.3	9
74	A global coupled cluster potential energy surface for HCl + OH â†" Cl + H₂O. Physical Chemistry Chemical Physics, 2017, 19, 9770-9777.	1.3	19
75	Three-Dimensional Diabatic Potential Energy Surfaces for the Photodissociation of Thiophenol. Journal of Physical Chemistry A, 2017, 121, 8432-8439.	1.1	17
76	Nanoparticle encapsulation in vesicles formed by amphiphilic diblock copolymers. Soft Matter, 2017, 13, 7840-7847.	1.2	21
77	Accurate Determination of Tunneling-Affected Rate Coefficients: Theory Assessing Experiment. Journal of Physical Chemistry Letters, 2017, 8, 3392-3397.	2.1	22
78	Rate Coefficients of the HCl + OH â†' Cl + H₂O Reaction from Ring Polymer Molecular Dynamics. Journal of Physical Chemistry A, 2016, 120, 3433-3440.	1.1	36
79	Nonadiabatic Tunneling in Photodissociation of Phenol. Journal of the American Chemical Society, 2016, 138, 7828-7831.	6.6	126
80	Amide Rotation Hindrance Predicts Proteolytic Resistance of Cystine-Knot Peptides. Journal of Physical Chemistry Letters, 2016, 7, 1138-1142.	2.1	6
81	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
82	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
83	Communication: On the competition between adiabatic and nonadiabatic dynamics in vibrationally mediated ammonia photodissociation in its A band. Journal of Chemical Physics, 2015, 142, 091101.	1.2	30
84	Signatures of non-adiabatic dynamics in the fine-structure state distributions of the OH(XÌƒ/AÌƒ) products in the B-band photodissociation of H2O. Journal of Chemical Physics, 2015, 142, 124317.	1.2	23
85	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
86	Stateâ€toâ€state reaction dynamics for the reactions of atom N with radicals. International Journal of Quantum Chemistry, 2015, 115, 596-606.	1.0	1
87	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
88	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
89	Mechanistic Insights into a Classic Wonder Drugâ€"Aspirin. Journal of the American Chemical Society, 2015, 137, 70-73.	6.6	66
90	Full-Dimensional Quantum Dynamics of Vibrationally Mediated Photodissociation of NH₃ and ND₃ on Coupled Ab Initio Potential Energy Surfaces: Absorption Spectra and NH₂(Ãƒ²A₁)/NH₂(XÌƒ²B₁) Branching Ratios. Journal of Physical Chemistry A, 2014, 118, 11926-11934.	1.1	30

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91	A tribute to Guosen Yan. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	0
92	Product fine-structure resolved photodissociation dynamics: The A band of H2O. Journal of Chemical Physics, 2014, 140, 024310.	1.2	22
93	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
94	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
95	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
96	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
97	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
98	State-to-state quantum dynamics of the N(4S)Â+ÂC2($$ilde{X}$$ X ~ 1Î£+)Ââ†'ÂCN($$ilde{X}$$ X ~ 2Î£+)Â+ÂC(3P) reaction. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	2
99	Dissociative chemisorption dynamics of small molecules on metal surfaces. Science China Chemistry, 2014, 57, 87-99.	4.2	2
100	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
101	Interaction specific binding hotspots in Endonuclease colicin-immunity protein complex from MD simulations. Science China Chemistry, 2013, 56, 1143-1151.	4.2	7
102	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
103	Vibrationally mediated bond selective dissociative chemisorption of HOD on Cu(111). Chemical Science, 2013, 4, 503-508.	3.7	60
104	Mode selectivity in methane dissociative chemisorption on Ni(111). Chemical Science, 2013, 4, 3249.	3.7	115
105	Biomimetic membrane control of block copolymer vesicles with tunable wall thickness. Soft Matter, 2013, 9, 2434.	1.2	28
106	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
107	Influence of Step Defects on Methanol Decomposition: Periodic Density Functional Studies on Pd(211) and Kinetic Monte Carlo Simulations. Journal of Physical Chemistry C, 2013, 117, 451-459.	1.5	28
108	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

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109	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
110	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
111	A new six-dimensional potential energy surface for H2â€“N2O and its adiabatic-hindered-rotor treatment. Journal of Chemical Physics, 2013, 139, 034312.	1.2	28
112	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
113	State to state photodissociation dynamics of D2O in the B band. Journal of Chemical Physics, 2013, 139, 114303. Ab Initio Potential Energy Surfaces for Both the Ground (<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 562 Td (xmlns:mml="	1.2	14
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127	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
128	New ab initio potential energy surfaces for both the ground (Xl̀ƒ¹Aâ€²) and excited (Ãƒ¹Aâ€³) electronic states of HSiCl and the absorption and emission spectra of HSiCl/DSiCl. Journal of Computational Chemistry, 2011, 32, 1694-1702.	1.5	3
129	Superfluid response of 4HeNâ€“N2O clusters probed by path integral Monte Carlo simulations. Journal of Molecular Spectroscopy, 2011, 267, 136-143.	0.4	15
130	Initial steps in methanol steam reforming on PdZn and ZnO surfaces: Density functional theory studies. Surface Science, 2011, 605, 750-759.	0.8	58
131	A new ab initio potential energy surface and microwave and infrared spectra for the Neâ€“CO2 complex. Journal of Chemical Physics, 2010, 133, 104302.	1.2	31
132	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
133	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
134	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
135	N₂O in small paraâ€hydrogen clusters: Structures and energetics. Journal of Computational Chemistry, 2009, 30, 841-846.	1.5	5
136	Theoretical prediction of the noble gas complexes HeAuF and NeAuF. Science in China Series B: Chemistry, 2009, 52, 1987-1990.	0.8	10
137	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
138	Ab Initio Potential Energy Surfaces for the Ground (Xl̀ƒ1Aâ€²) and Excited (Ãƒ1Aâ€²â€²) Electronic States of HGeBr and the Absorption and Emission Spectra of HGeBr/DGeBr. Journal of Physical Chemistry A, 2009, 113, 7314-7321.	1.1	3
139	Theoretical study of adsorption and dissociation of NH3 on the Ir{110}(1Ã—2) surface. Science Bulletin, 2008, 53, 3169-3172.	4.3	5
140	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
141	First-principles study of decomposition of NH3 on Ir(100). Surface Science, 2008, 602, 1288-1294.	0.8	50
142	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
143	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
144	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

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145	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
146	Full-dimensional quantum dynamics of Aì*f*-state photodissociation of ammonia: Absorption spectra. Journal of Chemical Physics, 2008, 129, 154311.	1.2	29
147	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
148	Path integral Monte Carlo study of CO2 solvation in He4 clusters. Journal of Chemical Physics, 2008, 128, 224513.	1.2	17
149	Ab initio potential energy surfaces for both the ground (Xì*f*â€‰A1â€²) and excited (Aì*f*â€‰A1â€³) electronic states of HGeCl and the absorption and emission spectra of HGeCl/DGeCl. Journal of Chemical Physics, 2008, 129, 154313.	1.2	5
150	A DFT INVESTIGATION OF SULFUR ADSORPTION ON Ir(100). Journal of Theoretical and Computational Chemistry, 2007, 06, 177-185.	1.8	2
151	FIRST-PRINCIPLES STUDY OF ADSORPTION OF CN ON Cu(111). Journal of Theoretical and Computational Chemistry, 2007, 06, 523-529.	1.8	3
152	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
153	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
154	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
155	Supermolecule density functional calculations suggest a key role for solvent in alkaline hydrolysis of p-nitrophenyl phosphate. Chemical Communications, 2007, , 1638.	2.2	42
156	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
157	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
158	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
159	Global analytical potential energy surfaces for HO2(Xì*f*Aâ€³2) based on high-levelab initiocalculations. Journal of Chemical Physics, 2007, 126, 074315.	1.2	45
160	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
161	A computational investigation on the sequential rearrangement mechanism of 2-allyl-2,4,5-hexatrienaldehyde involving [1,5]-hydrogen migration and 8Ï€-electrocyclization. Journal of Computational Chemistry, 2007, 28, 2164-2169.	1.5	5
162	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	1.2	36

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