Pei-Yu Zhang

List of Publications by Year
in descending order

43 papers	1,107 citations	394286 19 h-index	395590 33 g-index
43 all docs	43 docs citations	43 times ranked	784 citing authors

#	Article	IF	Citations
1	Attosecond-resolution quantum dynamics calculations for atoms and molecules in strong laser fields. Physical Review E, 2008, 77, 066701.	0.8	227
2	Nonadiabatic ab initio molecular dynamics of photoisomerization in bridged azobenzene. Journal of Chemical Physics, 2012, 137, 204305.	1.2	54
3	Tuning peptide self-assembly by an in-tether chiral center. Science Advances, 2018, 4, eaar5907.	4.7	50
4	Overcoming the difficulties of predicting conformational polymorph energetics in molecular crystals via correlated wavefunction methods. Chemical Science, 2020, 11, 2200-2214.	3.7	48
5	Harnessing Cloud Architecture for Crystal Structure Prediction Calculations. Crystal Growth and Design, 2018, 18, 6891-6900.	1.4	41
6	Adiabatic/Nonadiabatic State-to-State Reactive Scattering Dynamics Implemented on Graphics Processing Units. Journal of Physical Chemistry A, 2013, 117, 8512-8518.	1.1	40
7	Theoretical investigation of the origin of the multipeak structure of kinetic-energy-release spectra from charge-resonance-enhanced ionization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msup><mml:mrow /><mml:mo>+</mml:mo></mml:msup></mml:mrow></mml:math>in intense laser fields. Physical Review A, 2011, 84, .	1.0	39
8	Exact quantum scattering study of the Ne+H2+ reaction on a new ab initio potential energy surface. Journal of Chemical Physics, 2010, 132, 014303.	1.2	38
9	Accurate high level ab initio-based global potential energy surface and dynamics calculations for ground state of CH2+. Journal of Chemical Physics, 2015, 142, 124302.	1.2	38
10	Exact quantum scattering study of the H + HS reaction on a new ab initio potential energy surface H2S (3A â€³). Journal of Chemical Physics, 2012, 136, 094308.	1.2	36
11	Dissociation and ionization competing processes for H2+ in intense laser field: Which one is larger?. Journal of Chemical Physics, 2012, 136, 024311.	1.2	35
12	Theoretical Determination of the Rate Coefficient for the HO_{2Â}+ HO₂ â†' H₂O₂+O₂ Reaction: Adiabatic Treatment of Anharmonic Torsional Effects. Journal of Physical Chemistry A, 2012, 116, 2089-2100.	1.1	35
13	An ab initio potential energy surface of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>He</mml:mtext><mml:mo>+</mml:mo><mml:msubsup><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow></mml:msubsup></mml:mrow></mml:math>Chemical Physics Letters, 2008, 464, 92-96.	1.2	28
14	Coriolis Coupling Effects in O⁺(⁴S) + H₂(X¹Î£_g⁺) â†' OH⁺(X³Î£^{â€“}) + H(²S) Reaction and Its Isotopic Variants: Exact Time-Dependent Quantum Scattering Study. Journal of Physical Chemistry A, 2012, 116, 10882-10888.	1.1	26
15	Prediction of the Relative Free Energies of Drug Polymorphs above Zero Kelvin. Crystal Growth and Design, 2020, 20, 5211-5224.	1.4	26
16	Quenching of OH(A2Î£+) by H2 through Conical Intersections: Highly Excited Products in Nonreactive Channel. Journal of Physical Chemistry A, 2010, 114, 6565-6568.	1.1	24
17	Photochemical dynamics simulations for transâ€“cis photoisomerizations of azobenzene and bridged azobenzene. Computational and Theoretical Chemistry, 2014, 1031, 13-21.	1.1	24
18	A Cloud Computing Platform for Scalable Relative and Absolute Binding Free Energy Predictions: New Opportunities and Challenges for Drug Discovery. Journal of Chemical Information and Modeling, 2021, 61, 2720-2732.	2.5	23

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19	Quantum State-to-State Dynamics of the H + LiH â†' H₂ + Li Reaction. Journal of Physical Chemistry A, 2015, 119, 8912-8921.	1.1	22
20	Spin-orbit effect in the energy pooling reaction O2(aÎ"1)+O2(aÎ"1)â†'O2(bÎ£1)+O2(XÎ£3). Journal of Chemical Physics, 2007, 126, 124304.	1.2	20
21	Computational Insights into Kinetic Hindrance Affecting Crystallization of Stable Forms of Active Pharmaceutical Ingredients. Crystal Growth and Design, 2020, 20, 1512-1525.	1.4	20
22	Nonadiabatic quantum reactive scattering of the OH(Aâ€‰Î£2+)+D2. Journal of Chemical Physics, 2010, 133, 174316.	1.2	18
23	Accurate Study on the Quantum Dynamics of the He + HeH⁺ (X¹Î£⁺) Reaction on A New ab Initio Potential Energy Surface for the Lowest 1¹Aâ€² Electronic Singlet State. Journal of Physical Chemistry A, 2013, 117, 1406-1412.	1.1	17
24	Direct multi-photon ionizations of H⁺₂in intense laser fields. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 085103.	0.6	16
25	Influence of collision energy on the dynamics of the reaction H (2S)Â+ÂNH (X3Î£â^')Ââ†'ÂN (4S)Â+ÂH2 (X1Î£ g +) by the state-to-state quantum mechanical study. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	16
26	<scp>GQSD</scp>: The program for the graphic processing units accelerated quantum scattering dynamics. International Journal of Quantum Chemistry, 2015, 115, 738-743.	1.0	14
27	Green Mechanochemical Strategy for the Discovery and Selective Preparation of Polymorphs of Active Pharmaceutical Ingredient Î³-Aminobutyric Acid (GABA). ACS Sustainable Chemistry and Engineering, 2020, 8, 16781-16790.	3.2	14
28	Full six-dimensional nonadiabatic quantum dynamics calculation for the energy pooling reaction O2(aÎ"1)+O2(aÎ"1)â†'O2(bÎ£1)+O2(XÎ£3). Journal of Chemical Physics, 2008, 128, 091103.	1.2	13
29	Quantum dynamical study of the electronic nonadiabaticity in the D + DBr â†' Br(Br*) + D2 reaction on new diabatic potential energy surfaces. Journal of Chemical Physics, 2012, 137, 194305.	1.2	13
30	Reactant Coordinate Based State-to-State Reactive Scattering Dynamics Implemented on Graphical Processing Units. Journal of Physical Chemistry A, 2014, 118, 8929-8935.	1.1	13
31	State-resolved differential and integral cross sections for the Ne + H2+ (v = 0â€"2, j = 0) â†' NeH+ + H reaction. Journal of Chemical Physics, 2016, 144, 184301.	1.2	11
32	Isotopic effect on the dynamics of the H/D + LiH/LiD reactions. Computational and Theoretical Chemistry, 2016, 1084, 188-195.	1.1	11
33	A fluorophore's electron-deficiency does matter in designing high-performance near-infrared fluorescent probes. Chemical Science, 2020, 11, 11205-11213.	3.7	10
34	Time-dependent Wave Packet Quantum Scattering Study of Reaction S(3P)+H2â†'HS+H on a New ab initio Potential Energy Surface 3Aâ€². Chinese Journal of Chemical Physics, 2012, 25, 291-296.	0.6	8
35	Quantum wave packet dynamics study of the S(3P)+H2 reaction on the lowest SH2(13Aâ€²â€²) state. Computational and Theoretical Chemistry, 2012, 997, 83-87.	1.1	7
36	Quantum wave packet calculation of the O(3P)+H2 reaction on the new potential energy surfaces for the two lowest states. Computational and Theoretical Chemistry, 2012, 986, 25-29.	1.1	6

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37	Time-dependent wave packet state-to-state quantum dynamics study of the abstraction reaction S(3P)+H2(v=0, j=0) on 13Aâ€³ electronic state. Chemical Physics, 2015, 453-454, 47-53.	0.9	5
38	Photoisomerization mechanism of 1,1â€²-dimethyl-2,2â€²-pyridocyanine in the gas phase and in solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 1157-1166.	2.0	5
39	Exact Quantum-Scattering Study of the D(2 S)+DS(2 Î) Reaction. Chinese Physics Letters, 2012, 29, 073401.	1.3	4
40	Hybrid many-body-expansion/Shepard-interpolation method for constructing ab initio potential energy surfaces for quantum dynamics calculations. Chemical Physics Letters, 2013, 556, 393-397.	1.2	4
41	A THEORETICAL ANALYSIS OF THE DISSOCIATION OF OH RADICAL: FINE-STRUCTURE DISTRIBUTIONS OF THE O(3PJ) PRODUCT. Journal of Theoretical and Computational Chemistry, 2011, 10, 747-767.	1.8	3
42	Time-Dependent Wave-Packet Quantum Dynamics Study of the Ne + D₂⁺ (v₀ = 0â€“2, j₀ = 0) â†’ NeD⁺ + D Reaction: Including the Coriolis Coupling. Journal of Physical Chemistry A, 2014, 118, 5076-5082.	1.1	3
43	Quantum dynamics study on the exchange H+OH+ reaction. Computational and Theoretical Chemistry, 2013, 1012, 1-7.	1.1	2