Zhaojun Zhang

List of Publications by Year
in descending order

33	873	623574 14	477173 29
papers	citations	h-index	g-index

33	33	33	431
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Infrared Spectroscopy of Stepwise Hydration Motifs of Sulfur Dioxide. Journal of Physical Chemistry Letters, 2022, 13, 5654-5659.	2.1	8
2	Vibrational Signature of Dynamic Coupling of a Strong Hydrogen Bond. Journal of Physical Chemistry Letters, 2021, 12, 2259-2265.	2.1	12
3	Full-dimensional quantum dynamics study of isotope effects for the H2 + NH2/ND2/NHD and H2/D2/HD + NH2 reactions. Journal of Chemical Physics, 2021, 154, 074301.	1.2	0
4	A thermodynamics study of hydrogen interaction with (1 1 0) transition metal surfaces. Applied Surface Science, 2021, 545, 148961.	3.1	6
5	Theoretical new insights into hydrogen interaction with single-atom Zn- and co-doped copper metal catalysts. Applied Surface Science, 2021, 551, 149365.	3.1	2
6	Methane activation on single-atom Ir-doped metal nanoparticles from first principles. Physical Chemistry Chemical Physics, 2021, 23, 15564-15573.	1.3	10
7	Deconstructing Vibrational Motions on the Potential Energy Surfaces of Hydrogen-Bonded Complexes. CCS Chemistry, 2021, 3, 829-835.	4.6	13
8	A full-dimensional ab initio potential energy and dipole moment surfaces for (NH3)2. Journal of Chemical Physics, 2021, 155, 164306.	1.2	1
9	Exclusive Neural Network Representation of the Quasi-Diabatic Hamiltonians Including Conical Intersections. Journal of Physical Chemistry Letters, 2020, 11, 7552-7558.	2.1	16
10	Hot-Atom Mechanism in Syngas Methanation on Precovered Pd(100) Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 5312-5317.	2.1	9
11	Infrared Spectroscopy of Neutral Water Dimer Based on a Tunable Vacuum Ultraviolet Free Electron Laser. Journal of Physical Chemistry Letters, 2020, 11, 851-855.	2.1	50
12	Dissociative chemisorption of O2 on Agn and Agnâ^'1Ir (n = 3â€“26) clusters: a first-principle study. Physical Chemistry Chemical Physics, 2020, 22, 9053-9066.	1.3	11
13	Full-dimensional quantum mechanical calculations of the reaction probability of the H + CH4 reaction based on a mixed Jacobi and Radau description. Journal of Chemical Physics, 2020, 152, 201101.	1.2	14
14	Full dimensional quantum mechanical calculations of the reaction probability of the H + NH3 collision based on a mixed Jacobi and Radau description. Journal of Chemical Physics, 2019, 150, 204301.	1.2	12
15	Computing energy levels of CH4, CHD3, CH3D, and CH3F with a direct product basis and coordinates based on the methyl subsystem. Journal of Chemical Physics, 2018, 148, 074113.	1.2	7
16	Water dissociating on rigid Ni(100): A quantum dynamics study on a full-dimensional potential energy surface. Journal of Chemical Physics, 2018, 148, 144705.	1.2	20
17	Well converged quantum rate constants for the H2+ OH â†' H2O + H reaction via transition state wave packet. Journal of Chemical Physics, 2018, 149, 064303.	1.2	12
18	Dynamical barrier and isotope effects in the simplest substitution reaction via Walden inversion mechanism. Nature Communications, 2017, 8, 14506.	5.8	18

#	Article	IF	Citations
19	Methane dissociation on Ni(111): A seven-dimensional to nine-dimensional quantum dynamics study. Journal of Chemical Physics, 2017, 147, 024702.	1.2	8
20	Full-dimensional vibrational calculations of five-atom molecules using a combination of Radau and Jacobi coordinates: Applications to methane and fluoromethane. Journal of Chemical Physics, 2016, 144, 204302.	1.2	15
21	First-principles quantum dynamical theory for the dissociative chemisorption of H2O on rigid Cu(111). Nature Communications, 2016, 7, 11953.	5.8	74
22	Communication: Methane dissociation on Ni(111) surface: Importance of azimuth and surface impact site. Journal of Chemical Physics, 2016, 144, 101101.	1.2	30
23	Eight-Dimensional Quantum Dynamics Study of CH₄ and CD₄ Dissociation on Ni(100) Surface. Journal of Physical Chemistry C, 2016, 120, 20199-20205.	1.5	12
24	A seven-dimensional quantum dynamics study of the dissociative chemisorption of H₂O on Cu(111): effects of azimuthal angles and azimuthal angle-averaging. Chemical Science, 2016, 7, 1840-1845.	3.7	64
25	Mode specificity for the dissociative chemisorption of H₂O on Cu(111): a quantum dynamics study on an accurately fitted potential energy surface. Physical Chemistry Chemical Physics, 2016, 18, 8537-8544.	1.3	33
26	Methane dissociation on Ni(111): A fifteen-dimensional potential energy surface using neural network method. Journal of Chemical Physics, 2015, 143, 144701.	1.2	68
27	CH₄ dissociation on Ni(111): a quantum dynamics study of lattice thermal motion. Physical Chemistry Chemical Physics, 2015, 17, 25499-25504.	1.3	41
28	Time-Dependent Wave Packet Study of the H₂ + CH₃ â†' H + CH₄ Reaction. Journal of Physical Chemistry A, 2015, 119, 12480-12484.	1.1	9
29	Accuracy of the centrifugal sudden approximation in the H + CHD3 â†' H2 + CD3 reaction. Journal of Chemical Physics, 2014, 140, 224304.	1.2	41
30	Effects of reagent rotational excitation on the H + CHD3 â†' H2 + CD3 reaction: A seven dimensional time-dependent wave packet study. Journal of Chemical Physics, 2014, 141, 144309.	1.2	50
31	Communication: A six-dimensional state-to-state quantum dynamics study of the H + CH4 â†' H2 + CH3 reaction (J = 0). Journal of Chemical Physics, 2013, 138, 011101.	1.2	49
32	Theoretical Study of the Validity of the Polanyi Rules for the Late-Barrier Cl + CHD₃ Reaction. Journal of Physical Chemistry Letters, 2012, 3, 3416-3419.	2.1	106
33	Total Synthesis of the Antiallergic Naphtho-Î±-pyrone Tetraglucoside, Cassiaside C2, Isolated from Cassia Seeds. Journal of Organic Chemistry, 2003, 68, 6309-6313.	1.7	52