Xuefei Xu

List of Publications by Year
in descending order

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65 papers	3,216 citations	218381 26 h-index	155451 55 g-index
66 all docs	66 docs citations	66 times ranked	3951 citing authors

#	Article	IF	Citations
1	Minimally augmented Karlsruhe basis sets. Theoretical Chemistry Accounts, 2011, 128, 295-305.	0.5	638
2	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. Journal of Chemical Theory and Computation, 2011, 7, 3027-3034.	2.3	566
3	How Well Can Modern Density Functionals Predict Internuclear Distances at Transition States?. Journal of Chemical Theory and Computation, 2011, 7, 1667-1676.	2.3	156
4	Adsorption on Fe-MOF-74 for C1â€“C3 Hydrocarbon Separation. Journal of Physical Chemistry C, 2013, 117, 12648-12660.	1.5	109
5	Do Practical Standard Coupled Cluster Calculations Agree Better than Kohnâ€“Sham Calculations with Currently Available Functionals When Compared to the Best Available Experimental Data for Dissociation Energies of Bonds to 3d Transition Metals?. Journal of Chemical Theory and Computation, 2015, 11, 2036-2052.	2.3	109
6	Photodissociation Dynamics of Phenol: Multistate Trajectory Simulations including Tunneling. Journal of the American Chemical Society, 2014, 136, 16378-16386.	6.6	102
7	Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures. Journal of the American Chemical Society, 2018, 140, 2906-2918.	6.6	100
8	Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. Chemical Science, 2014, 5, 4661-4680.	3.7	90
9	Accuracy of Effective Core Potentials and Basis Sets for Density Functional Calculations, Including Relativistic Effects, As Illustrated by Calculations on Arsenic Compounds. Journal of Chemical Theory and Computation, 2011, 7, 2766-2779.	2.3	78
10	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. Journal of Chemical Theory and Computation, 2014, 10, 102-121.	2.3	65
11	Single atom catalysts supported on N-doped graphene toward fast kinetics in Liâ€“S batteries: a theoretical study. Journal of Materials Chemistry A, 2021, 9, 12225-12235.	5.2	62
12	Diabatic Molecular Orbitals, Potential Energies, and Potential Energy Surface Couplings by the 4-fold Way for Photodissociation of Phenol. Journal of Chemical Theory and Computation, 2013, 9, 3612-3625.	2.3	61
13	Performance of Effective Core Potentials for Density Functional Calculations on 3d Transition Metals. Journal of Chemical Theory and Computation, 2012, 8, 80-90.	2.3	58
14	Diabatization based on the dipole and quadrupole: The DQ method. Journal of Chemical Physics, 2014, 141, 114104.	1.2	58
15	Methanol triggered ligand flip isomerization in a binuclear copper(i) complex and the luminescence response. Chemical Communications, 2011, 47, 9179.	2.2	52
16	Combined Self-Consistent-Field and Spin-Flip Tammâ€“Dancoff Density Functional Approach to Potential Energy Surfaces for Photochemistry. Journal of Physical Chemistry Letters, 2013, 4, 253-258.	2.1	50
17	Benchmark Calculations for Bond Dissociation Enthalpies of Unsaturated Methyl Esters and the Bond Dissociation Enthalpies of Methyl Linolenate. Journal of Physical Chemistry A, 2016, 120, 4025-4036.	1.1	49
18	Efficient Heteronuclear Diatom Electrocatalyst for Nitrogen Reduction Reaction: Pdâ€“Nb Diatom Supported on Black Phosphorus. ACS Applied Materials & Interfaces, 2020, 12, 56987-56994.	4.0	49

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19	Ligand- and Anion-Controlled Formation of Silver Alkynyl Oligomers from Soluble Precursors. Inorganic Chemistry, 2008, 47, 1877-1879.	1.9	45
20	Configuration Interaction-Corrected Tammâ€“Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. Journal of Physical Chemistry Letters, 2014, 5, 322-328.	2.1	45
21	Direct diabatization of electronic states by the fourfold-way: Including dynamical correlation by multi-configuration quasidegenerate perturbation theory with complete active space self-consistent-field diabatic molecular orbitals. Chemical Physics Letters, 2013, 573, 84-89.	1.2	42
22	Molecular Symmetry Properties of Conical Intersections and Nonadiabatic Coupling Terms: Theory and Quantum Chemical Demonstration for Cyclopenta-2,4-dienimine (C5H4NH). Journal of Physical Chemistry A, 2010, 114, 2991-3010.	1.1	33
23	Multi-structural variational transition state theory: kinetics of the 1,5-hydrogen shift isomerization of the 1-butoxyl radical including all structures and torsional anharmonicity. Physical Chemistry Chemical Physics, 2012, 14, 4204.	1.3	33
24	Testing Noncollinear Spin-Flip, Collinear Spin-Flip, and Conventional Time-Dependent Density Functional Theory for Predicting Electronic Excitation Energies of Closed-Shell Atoms. Journal of Chemical Theory and Computation, 2014, 10, 2070-2084.	2.3	33
25	Photoreactivity of a Pushâ^'Pull Merocyanine in Static Electric Fields: A Three-State Model of Isomerization Reactions Involving Conical Intersections. Journal of Physical Chemistry A, 2009, 113, 9779-9791.	1.1	32
26	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. ACS Catalysis, 2015, 5, 2070-2080.	5.5	28
27	Quantum Mechanical Fragment Methods Based on Partitioning Atoms or Partitioning Coordinates. Accounts of Chemical Research, 2014, 47, 2731-2738.	7.6	27
28	Electrophilic Aromatic Substitution: The Role of Electronically Excited States. Journal of Physical Chemistry A, 2010, 114, 4924-4933.	1.1	25
29	Multistructural Variational Transition State Theory: Kinetics of the Hydrogen Abstraction from Carbon-2 of 2-Methyl-1-propanol by Hydroperoxyl Radical Including All Structures and Torsional Anharmonicity. Journal of Physical Chemistry A, 2012, 116, 10480-10487.	1.1	24
30	Army ants tunneling for classical simulations. Chemical Science, 2014, 5, 2091-2099.	3.7	24
31	Predicting bond dissociation energy and bond length for bimetallic diatomic molecules: a challenge for electronic structure theory. Physical Chemistry Chemical Physics, 2017, 19, 5839-5854.	1.3	21
32	Computational Characterization of Low-Lying States and Intramolecular Charge Transfers in N-Phenylpyrrole and the Planar-Rigidized Fluorazene. Journal of Physical Chemistry A, 2006, 110, 1740-1748.	1.1	20
33	Theoretical Study on the Singlet Excited State of Pterin and Its Deactivation Pathway. Journal of Physical Chemistry A, 2007, 111, 9255-9262.	1.1	20
34	Theoretical study of photoinduced singlet and triplet excited states of 4-dimethylaminobenzonitrile and its derivatives. Journal of Chemical Physics, 2005, 122, 194305.	1.2	19
35	Ultraviolet Absorption Spectrum of Malonaldehyde in Water Is Dominated by Solvent-Stabilized Conformations. Journal of the American Chemical Society, 2015, 137, 8026-8029.	6.6	18
36	Nonintuitive Diabatic Potential Energy Surfaces for Thioanisole. Journal of Physical Chemistry Letters, 2015, 6, 3352-3359.	2.1	17

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37	Computational Kinetics by Variational Transition-State Theory with Semiclassical Multidimensional Tunneling: Direct Dynamics Rate Constants for the Abstraction of H from CH3OH by Triplet Oxygen Atoms. Journal of Physical Chemistry A, 2017, 121, 1693-1707.	1.1	17
38	Anchor Points Reactive Potential for Bond-Breaking Reactions. Journal of Chemical Theory and Computation, 2014, 10, 924-933.	2.3	16
39	Computational simulation and interpretation of the low-lying excited electronic states and electronic spectrum of thioanisole. Physical Chemistry Chemical Physics, 2015, 17, 20093-20099.	1.3	16
40	Kinetics of the Toluene Reaction with OH Radical. Research, 2019, 2019, 5373785.	2.8	16
41	Thermochemistry of radicals formed by hydrogen abstraction from 1-butanol, 2-methyl-1-propanol, and butanal. Journal of Chemical Physics, 2012, 137, 104314.	1.2	15
42	Nonmonotonic Temperature Dependence of the Pressure-Dependent Reaction Rate Constant and Kinetic Isotope Effect of Hydrogen Radical Reaction with Benzene Calculated by Variational Transition-State Theory. Journal of Physical Chemistry A, 2017, 121, 9033-9044.	1.1	15
43	Computational kinetics of the hydrogen abstraction reactions of n-propanol and iso-propanol by OH radical. Physical Chemistry Chemical Physics, 2019, 21, 24458-24468.	1.3	15
44	Quantum Effects on H₂ Diffusion in Zeolite RHO: Inverse Kinetic Isotope Effect for Sieving. Journal of the American Chemical Society, 2019, 141, 13635-13642.	6.6	14
45	Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. Angewandte Chemie - International Edition, 2020, 59, 10826-10830.	7.2	13
46	INTRAMOLECULAR CHARGE TRANSFER AND PHOTOISOMERIZATION OF THE DCM STYRENE DYE: A THEORETICAL STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 719-736.	1.8	12
47	Accurate entropy calculation for large flexible hydrocarbons using a multi-structural 2-dimensional torsion method. Physical Chemistry Chemical Physics, 2019, 21, 10003-10010.	1.3	12
48	Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. Angewandte Chemie, 2020, 132, 10918-10922.	1.6	10
49	Understanding the Separation Mechanism of C2H6/C2H4 on Zeolitic Imidazolate Framework ZIF-7 by Periodic DFT Investigations. Journal of Physical Chemistry C, 2020, 124, 256-266.	1.5	9
50	TUMME: Tsinghua University Minnesota Master Equation program. Computer Physics Communications, 2022, 270, 108140.	3.0	8
51	How sodium chloride extends lifetime of bulk nanobubbles in water. Soft Matter, 2022, 18, 2968-2978.	1.2	8
52	Mechanistic Study on Enhanced Electrocatalytic Nitrogen Reduction Reaction by Mo Single Clusters Supported on MoS₂. ACS Applied Materials & Interfaces, 2022, 14, 28900-28910.	4.0	8
53	Large Anharmonic Effects on Tunneling and Kinetics: Reaction of Propane with Muonium. Journal of Physical Chemistry Letters, 2021, 12, 4154-4159.	2.1	7
54	Low-Pressure Limit of Competitive Unimolecular Reactions. Journal of the American Chemical Society, 2020, 142, 16064-16071.	6.6	6

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55	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadiumâ€“Ligand Bonds. Journal of Physical Chemistry A, 2020, 124, 9757-9770.	1.1	5
56	Pressure-dependent kinetics of the o-xylene reaction with OH radicals. Physical Chemistry Chemical Physics, 2022, 24, 8672-8682.	1.3	5
57	A kinetics study on hydrogen abstraction reactions of cyclopentane by hydrogen, methyl, and ethyl radicals. Physical Chemistry Chemical Physics, 2021, 23, 7333-7342.	1.3	4
58	Mechanistic Insights into Electrocatalytic Nitrogen Reduction Reaction on the Pdâ€W Heteronuclear Diatom Supported on C₂N Monolayer: Role of H Preâ€Adsorption. Energy and Environmental Materials, 2023, 6, .	7.3	4
59	Master equation study of hydrogen abstraction from HCHO by OH via a chemically activated intermediate. Faraday Discussions, 0, 238, 431-460.	1.6	4
60	Observing Intramolecular Vibrational Energy Redistribution via the Short-Time Fourier Transform. Journal of Physical Chemistry A, 2022, 126, 3006-3014.	1.1	4
61	What Definitively Controls the Photochemical Activity of Methylbenzonitriles and Methylanisoles? Insights from Theory. Journal of Physical Chemistry A, 2007, 111, 5775-5783.	1.1	3
62	A chemically consistent rate constant for the reaction of nitrogen dioxide with the oxygen atom. Physical Chemistry Chemical Physics, 2021, 23, 585-596.	1.3	3
63	Energy Dependence of Ensemble-Averaged Energy Transfer Moments and Its Effect on Competing Decomposition Reactions. Journal of Physical Chemistry A, 2021, 125, 6303-6313.	1.1	3
64	Self-diffusion mechanisms based defect complexes in MoSi₂. Journal of Physics Condensed Matter, 2021, 33, 465402.	0.7	3
65	gâ€C ₃ N ₄ â€Supported Metalâ€Pair Catalysts toward Efficient Electrocatalytic Nitrogen Reduction: A Computational Evaluation. Advanced Theory and Simulations, 0, , 2100579.	1.3	2