Xuefei Xu

List of Publications by Year in Descending Order

58 papers	2,341 citations	24 h-index	48 g-index
66 ext. papers	2,739 ext. citations	6.2 avg, IF	5.35 L-index

#	Paper	IF	Citations
58	TUMME: Tsinghua University Minnesota Master Equation program. *Computer Physics Communications*, **2022**, 270, 108140	4.2	2
57	Large Anharmonic Effects on Tunneling and Kinetics: Reaction of Propane with Muonium. *Journal of Physical Chemistry Letters*, **2021**, 12, 4154-4159	6.4	3
56	A chemically consistent rate constant for the reaction of nitrogen dioxide with the oxygen atom. *Physical Chemistry Chemical Physics*, **2021**, 23, 585-596	3.6	1
55	Single atom catalysts supported on N-doped graphene toward fast kinetics in Li‒S batteries: a theoretical study. *Journal of Materials Chemistry A*, **2021**, 9, 12225-12235	13	18
54	A kinetics study on hydrogen abstraction reactions of cyclopentane by hydrogen, methyl, and ethyl radicals. *Physical Chemistry Chemical Physics*, **2021**, 23, 7333-7342	3.6	1
53	Energy Dependence of Ensemble-Averaged Energy Transfer Moments and Its Effect on Competing Decomposition Reactions. *Journal of Physical Chemistry A*, **2021**, 125, 6303-6313	2.8	0
52	Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. *Angewandte Chemie*, **2020**, 132, 10918-10922	3.6	5
51	Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. *Angewandte Chemie - International Edition*, **2020**, 59, 10826-10830	16.4	7
50	Efficient Heteronuclear Diatom Electrocatalyst for Nitrogen Reduction Reaction: Pd-Nb Diatom Supported on Black Phosphorus. *ACS Applied Materials & Interfaces*, **2020**, 12, 56987-56994	9.5	19
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	3.8	3
48	Predicting Bond Dissociation Energies and Bond Lengths of Coordinatively Unsaturated Vanadium-Ligand Bonds. *Journal of Physical Chemistry A*, **2020**, 124, 9757-9770	2.8	3
47	Low-Pressure Limit of Competitive Unimolecular Reactions. *Journal of the American Chemical Society*, **2020**, 142, 16064-16071	16.4	2
46	Accurate entropy calculation for large flexible hydrocarbons using a multi-structural 2-dimensional torsion method. *Physical Chemistry Chemical Physics*, **2019**, 21, 10003-10010	3.6	7
45	Quantum Effects on H Diffusion in Zeolite RHO: Inverse Kinetic Isotope Effect for Sieving. *Journal of the American Chemical Society*, **2019**, 141, 13635-13642	16.4	7
44	Kinetics of the Toluene Reaction with OH Radical. *Research*, **2019**, 2019, 5373785	7.8	8
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	3.6	8
42	Kinetics of the Methanol Reaction with OH at Interstellar, Atmospheric, and Combustion Temperatures. *Journal of the American Chemical Society*, **2018**, 140, 2906-2918	16.4	61

41	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	3.6	16
40	Computational Kinetics by Variational Transition-State Theory with Semiclassical Multidimensional Tunneling: Direct Dynamics Rate Constants for the Abstraction of H from CHOH by Triplet Oxygen Atoms. *Journal of Physical Chemistry A*, **2017**, 121, 1693-1707	2.8	9
39	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	2.8	8
38	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, 4025-36	2.8	36
37	Computational simulation and interpretation of the low-lying excited electronic states and electronic spectrum of thioanisole. *Physical Chemistry Chemical Physics*, **2015**, 17, 20093-9	3.6	14
36	Ultraviolet Absorption Spectrum of Malonaldehyde in Water Is Dominated by Solvent-Stabilized Conformations. *Journal of the American Chemical Society*, **2015**, 137, 8026-9	16.4	15
35	Do Practical Standard Coupled Cluster Calculations Agree Better than Kohn-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, 2036-52	6.4	91
34	Nonintuitive Diabatic Potential Energy Surfaces for Thioanisole. *Journal of Physical Chemistry Letters*, **2015**, 6, 3352-9	6.4	15
33	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. *ACS Catalysis*, **2015**, 5, 2070-2080	13.1	25
32	Anchor Points Reactive Potential for Bond-Breaking Reactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 924-33	6.4	15
31	Density Functional Theory of Open-Shell Systems. The 3d-Series Transition-Metal Atoms and Their Cations. *Journal of Chemical Theory and Computation*, **2014**, 10, 102-21	6.4	55
30	Configuration Interaction-Corrected Tamm-Dancoff Approximation: A Time-Dependent Density Functional Method with the Correct Dimensionality of Conical Intersections. *Journal of Physical Chemistry Letters*, **2014**, 5, 322-8	6.4	40
29	Diabatization based on the dipole and quadrupole: the DQ method. *Journal of Chemical Physics*, **2014**, 141, 114104	3.9	50
28	Photodissociation dynamics of phenol: multistate trajectory simulations including tunneling. *Journal of the American Chemical Society*, **2014**, 136, 16378-86	16.4	88
27	Full-dimensional potentials and state couplings and multidimensional tunneling calculations for the photodissociation of phenol. *Chemical Science*, **2014**, 5, 4661-4680	9.4	80
26	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, 2070-84	6.4	28
25	Army ants tunneling for classical simulations. *Chemical Science*, **2014**, 5, 2091-2099	9.4	22
24	Quantum mechanical fragment methods based on partitioning atoms or partitioning coordinates. *Accounts of Chemical Research*, **2014**, 47, 2731-8	24.3	20

23	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	2.5	37
22	Adsorption on Fe-MOF-74 for C1C3 Hydrocarbon Separation. *Journal of Physical Chemistry C*, **2013**, 117, 12648-12660	3.8	94
21	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, 3612-25	6.4	54
20	Combined Self-Consistent-Field and Spin-Flip Tamm-Dancoff Density Functional Approach to Potential Energy Surfaces for Photochemistry. *Journal of Physical Chemistry Letters*, **2013**, 4, 253-8	6.4	41
19	Performance of Effective Core Potentials for Density Functional Calculations on 3d Transition Metals. *Journal of Chemical Theory and Computation*, **2012**, 8, 80-90	6.4	52
18	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, 4204-16	3.6	31
17	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, 10480-7	2.8	23
16	Thermochemistry of radicals formed by hydrogen abstraction from 1-butanol, 2-methyl-1-propanol, and butanal. *Journal of Chemical Physics*, **2012**, 137, 104314	3.9	10
15	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, 2766-79	6.4	58
14	Perspectives on Basis Sets Beautiful: Seasonal Plantings of Diffuse Basis Functions. *Journal of Chemical Theory and Computation*, **2011**, 7, 3027-34	6.4	393
13	How Well Can Modern Density Functionals Predict Internuclear Distances at Transition States?. *Journal of Chemical Theory and Computation*, **2011**, 7, 1667-76	6.4	140
12	Minimally augmented Karlsruhe basis sets. *Theoretical Chemistry Accounts*, **2011**, 128, 295-305	1.9	388
11	Methanol triggered ligand flip isomerization in a binuclear copper(I) complex and the luminescence response. *Chemical Communications*, **2011**, 47, 9179-81	5.8	46
10	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	2.8	31
9	Electrophilic aromatic substitution: the role of electronically excited states. *Journal of Physical Chemistry A*, **2010**, 114, 4924-33	2.8	22
8	Photoreactivity of a push-pull merocyanine in static electric fields: a three-state model of isomerization reactions involving conical intersections. *Journal of Physical Chemistry A*, **2009**, 113, 9779-91	2.8	29
7	Ligand- and anion-controlled formation of silver alkynyl oligomers from soluble precursors. *Inorganic Chemistry*, **2008**, 47, 1877-9	5.1	43
6	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	10

5	What definitively controls the photochemical activity of methylbenzonitriles and methylanisoles? Insights from theory. *Journal of Physical Chemistry A*, **2007**, 111, 5775-83	2.8	2
4	Theoretical study on the singlet excited state of pterin and its deactivation pathway. *Journal of Physical Chemistry A*, **2007**, 111, 9255-62	2.8	17
3	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, 1740-8	2.8	20
2	Theoretical study of photoinduced singlet and triplet excited states of 4-dimethylaminobenzonitrile and its derivatives. *Journal of Chemical Physics*, **2005**, 122, 194305	3.9	15
1	g-C 3 N 4 -Supported Metal-Pair Catalysts toward Efficient Electrocatalytic Nitrogen Reduction: A Computational Evaluation. *Advanced Theory and Simulations*,2100579	3.5	0