Joseph Francisco

List of Publications by Year
in descending order

409	12,490	57	87
papers	citations	h-index	g-index
		24978	49773

424	424	424	9558
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical studies of atmospheric reaction mechanisms in the troposphere. Chemical Society Reviews, 2012, 41, 6259.	18.7	360
2	Water Catalysis of a Radical-Molecule Gas-Phase Reaction. Science, 2007, 315, 497-501.	6.0	299
3	Rational Design of Flexible Two-Dimensional MXenes with Multiple Functionalities. Chemical Reviews, 2019, 119, 11980-12031.	23.0	242
4	Promising electron mobility and high thermal conductivity in Sc₂CT₂(T = F,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.8	205
5	Kinetics and Mechanisms of Aqueous Ozone Reactions with Bromide, Sulfite, Hydrogen Sulfite, Iodide, and Nitrite Ions. Inorganic Chemistry, 2001, 40, 4436-4442.	1.9	187
6	Radicalâˆ’Water Complexes in Earth's Atmosphere. Accounts of Chemical Research, 2000, 33, 825-830.	7.6	178
7	The thermal and electrical properties of the promising semiconductor MXene Hf2CO2. Scientific Reports, 2016, 6, 27971.	1.6	178
8	Single Iridium Atom Doped Ni₂P Catalyst for Optimal Oxygen Evolution. Journal of the American Chemical Society, 2021, 143, 13605-13615.	6.6	162
9	Existence of a Hydroperoxy and Water (HO2Â·H2O) Radical Complex. Journal of Physical Chemistry A, 1998, 102, 1899-1902.	1.1	155
10	In Situ Observation of the pH Gradient near the Gas Diffusion Electrode of CO₂ Reduction in Alkaline Electrolyte. Journal of the American Chemical Society, 2020, 142, 15438-15444.	6.6	154
11	Atomic imaging of the edge structure and growth of a two-dimensional hexagonal ice. Nature, 2020, 577, 60-63.	13.7	149
12	Molecular reactions at aqueous interfaces. Nature Reviews Chemistry, 2020, 4, 459-475.	13.8	149
13	Stabilization and strengthening effects of functional groups in two-dimensional titanium carbide. Physical Review B, 2016, 94, .	1.1	142
14	Intrinsic Structural, Electrical, Thermal, and Mechanical Properties of the Promising Conductor Mo₂C MXene. Journal of Physical Chemistry C, 2016, 120, 15082-15088.	1.5	139
15	Rational Design of Highly Stable and Active MXeneâ€Based Bifunctional ORR/OER Doubleâ€Atom Catalysts. Advanced Materials, 2021, 33, e2102595.	11.1	137
16	Distinct ice patterns on solid surfaces with various wettabilities. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11285-11290.	3.3	132
17	Integrating Rh Species with NiFe-Layered Double Hydroxide for Overall Water Splitting. Nano Letters, 2020, 20, 136-144.	4.5	129
18	Sulfuric Acid as Autocatalyst in the Formation of Sulfuric Acid. Journal of the American Chemical Society, 2012, 134, 20632-20644.	6.6	126

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19	Water effects on atmospheric reactions. International Reviews in Physical Chemistry, 2011, 30, 335-369.	0.9	119
20	The <i>trans</i>-HOCO radical: Quartic force fields, vibrational frequencies, and spectroscopic constants. Journal of Chemical Physics, 2011, 135, 134301.	1.2	116
21	New Mechanistic Pathways for Criegeeâ€“Water Chemistry at the Air/Water Interface. Journal of the American Chemical Society, 2016, 138, 11164-11169.	6.6	111
22	HOCO Radical Chemistry. Accounts of Chemical Research, 2010, 43, 1519-1526.	7.6	109
23	Quartic force field predictions of the fundamental vibrational frequencies and spectroscopic constants of the cations HOCO+ and DOCO+. Journal of Chemical Physics, 2012, 136, 234309.	1.2	105
24	Experimental Evidence for the Existence of the HO2âˆ™H2O Complex. Journal of Physical Chemistry A, 2000, 104, 6597-6601.	1.1	104
25	Atmospheric Significance of Water Clusters and Ozoneâ€“Water Complexes. Journal of Physical Chemistry A, 2013, 117, 10381-10396.	1.1	101
26	Insight into Chemistry on Cloud/Aerosol Water Surfaces. Accounts of Chemical Research, 2018, 51, 1229-1237.	7.6	96
27	Coupled Cluster Theory Determination of the Heats of Formation of Combustion-Related Compounds:Â CO, HCO, CO2, HCO2, HOCO, HC(O)OH, and HC(O)OOH. Journal of Physical Chemistry A, 2003, 107, 1604-1617.	1.1	94
28	An Investigation of the Factors Influencing Student Performance in Physical Chemistry. Journal of Chemical Education, 2001, 78, 99.	1.1	93
29	Near-Barrierless Ammonium Bisulfate Formation via a Loop-Structure Promoted Proton-Transfer Mechanism on the Surface of Water. Journal of the American Chemical Society, 2016, 138, 1816-1819.	6.6	93
30	Impact of Water on the OH + HOCl Reaction. Journal of the American Chemical Society, 2011, 133, 3345-3353.	6.6	92
31	The Isomerization of Methoxy Radical: Intramolecular Hydrogen Atom Transfer Mediated through Acid Catalysis. Journal of the American Chemical Society, 2011, 133, 2013-2015.	6.6	91
32	Effects of a Single Water Molecule on the OH + H₂O₂ Reaction. Journal of Physical Chemistry A, 2012, 116, 5821-5829.	1.1	91
33	Interconnection of Reactive Oxygen Species Chemistry across the Interfaces of Atmospheric, Environmental, and Biological Processes. Accounts of Chemical Research, 2015, 48, 575-583.	7.6	90
34	Characterizing hydrophobicity of amino acid side chains in a protein environment via measuring contact angle of a water nanodroplet on planar peptide network. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12946-12951.	3.3	87
35	Self-Catalytic Reaction of SO₃ and NH₃ To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. Journal of the American Chemical Society, 2018, 140, 11020-11028.	6.6	86
36	Effect of Irradiation Sources and Oxygen Concentration on the Photocatalytic Oxidation of 2-Propanol and Acetone Studied by in Situ FTIR. Journal of Physical Chemistry B, 2003, 107, 4537-4544.	1.2	84

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37	Multielemental singleâ€“atom-thick <i>A</i> layers in nanolaminated V ₂ (Sn, <i>A</i>) C () Tj ETQq1 1 0.784314 rgBT / Sciences of the United States of America, 2020, 117, 820-825.	3.3	84
38	Structure, Anharmonic Vibrational Frequencies, and Intensities of NNHNN⁺. Journal of Physical Chemistry A, 2015, 119, 11623-11631.	1.1	81
39	Surprising Stability of Larger Criegee Intermediates on Aqueous Interfaces. Angewandte Chemie - International Edition, 2017, 56, 7740-7744.	7.2	80
40	Gas Phase Hydrolysis of Formaldehyde To Form Methanediol: Impact of Formic Acid Catalysis. Journal of Physical Chemistry A, 2013, 117, 11704-11710.	1.1	73
41	Ion-specific ice recrystallization provides a facile approach for the fabrication of porous materials. Nature Communications, 2017, 8, 15154.	5.8	71
42	Fundamental Vibrational Frequencies and Spectroscopic Constants of HOCS⁺, HSCO⁺, and Isotopologues via Quartic Force Fields. Journal of Physical Chemistry A, 2012, 116, 9582-9590.	1.1	70
43	Reactivity of Atmospherically Relevant Small Radicals at the Airâ€“Water Interface. Angewandte Chemie - International Edition, 2012, 51, 5413-5417.	7.2	69
44	Role of Double Hydrogen Atom Transfer Reactions in Atmospheric Chemistry. Accounts of Chemical Research, 2016, 49, 877-883.	7.6	69
45	The OH radical-H2O molecular interaction potential. Journal of Chemical Physics, 2006, 124, 224318.	1.2	67
46	Formation of HONO from the NH₃-promoted hydrolysis of NO₂dimers in the atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7236-7241.	3.3	67
47	Bond Dissociation Energies in Second-Row Compounds. Journal of Physical Chemistry A, 2008, 112, 3145-3156.	1.1	66
48	Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet. Journal of the American Chemical Society, 2012, 134, 11821-11827.	6.6	65
49	Assessing Student Understanding of General Chemistry with Concept Mapping. Journal of Chemical Education, 2002, 79, 248.	1.1	64
50	Hydrolysis of Glyoxal in Water-Restricted Environments: Formation of Organic Aerosol Precursors through Formic Acid Catalysis. Journal of Physical Chemistry A, 2014, 118, 4095-4105.	1.1	63
51	Mechanistic Study of the Gas-Phase Decomposition of Methyl Formate. Journal of the American Chemical Society, 2003, 125, 10475-10480.	6.6	62
52	Vibrational frequencies and spectroscopic constants from quartic force fields for <i>cis</i>-HOCO: The radical and the anion. Journal of Chemical Physics, 2011, 135, 214303.	1.2	62
53	Encapsulation kinetics and dynamics of carbon monoxide in clathrate hydrate. Nature Communications, 2014, 5, 4128.	5.8	62
54	Kinetics and Mechanism of the Acetylperoxy + HO2 Reaction. Journal of Physical Chemistry A, 1999, 103, 365-378.	1.1	60

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55	Exploring the OH+COâ†’H+CO2 potential surface via dissociative photodetachment of (HOCO)âˆ’. Journal of Chemical Physics, 2002, 117, 6478-6488.	1.2	60
56	A surface-stabilized ozonide triggers bromide oxidation at the aqueous solution-vapour interface. Nature Communications, 2017, 8, 700.	5.8	59
57	Infrared Spectrum and Stability of the H₂Oâˆ’HO Complex: Experiment and Theory. Journal of Physical Chemistry A, 2010, 114, 1529-1538.	1.1	58
58	Spectroscopic signatures of ozone at the airâ€“water interface and photochemistry implications. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11618-11623.	3.3	58
59	General-Acid-Catalyzed Reactions of Hypochlorous Acid and Acetyl Hypochlorite with Chlorite Ion. Inorganic Chemistry, 2000, 39, 2614-2620.	1.9	56
60	The importance of weak absorption features in promoting tropospheric radical production. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 7449-7452.	3.3	56
61	Water desalination through rim functionalized carbon nanotubes. Journal of Materials Chemistry A, 2019, 7, 3583-3591.	5.2	56
62	Unraveling the mechanism of selective ion transport in hydrophobic subnanometer channels. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10851-10856.	3.3	53
63	Reaction of Criegee Intermediate with Nitric Acid at the Airâ€“Water Interface. Journal of the American Chemical Society, 2018, 140, 4913-4921.	6.6	53
64	Heats of Formation of the H1,2OmSn (m, n = 0âˆ’3) Molecules from Electronic Structure Calculations. Journal of Physical Chemistry A, 2009, 113, 11343-11353.	1.1	52
65	Interaction of the NH₂ Radical with the Surface of a Water Droplet. Journal of the American Chemical Society, 2015, 137, 12070-12078.	6.6	52
66	Integrating Multiple Teaching Methods into a General Chemistry Classroom. Journal of Chemical Education, 1998, 75, 210.	1.1	51
67	Designing flexible 2D transition metal carbides with strain-controllable lithium storage. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E11082-E11091.	3.3	51
68	Nitric Acidâ€“Amine Chemistry in the Gas Phase and at the Airâ€“Water Interface. Journal of the American Chemical Society, 2018, 140, 6456-6466.	6.6	51
69	Existence of a Chlorine Oxide and Water (ClO.cntdot.H2O) Radical Complex. Journal of the American Chemical Society, 1995, 117, 9917-9918.	6.6	50
70	Making Sure That Hydrofluorocarbons Are â€œOzone Friendlyâ€ Accounts of Chemical Research, 1996, 29, 391-397.	7.6	50
71	Photochemistry of oxidized Hg(I) and Hg(II) species suggests missing mercury oxidation in the troposphere. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30949-30956.	3.3	50
72	Cavity Ringdown Spectroscopy of cis-cis HOONO and the HOONO/HONO2 Branching Ratio in the Reaction OH + NO2 + M. Journal of Physical Chemistry A, 2003, 107, 6974-6985.	1.1	48

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73	Hydrolysis of Ketene Catalyzed by Formic Acid: Modification of Reaction Mechanism, Energetics, and Kinetics with Organic Acid Catalysis. Journal of Physical Chemistry A, 2015, 119, 4347-4357.	1.1	48
74	Structure and Energetics of Hydrogen Bonded HOxâˆ'HNO3Complexes. Journal of Physical Chemistry A, 1999, 103, 6049-6053.	1.1	47
75	Uptake of the HO2radical by water: Molecular dynamics calculations and their implications for atmospheric modeling. Journal of Geophysical Research, 2004, 109, .	3.3	46
76	Interaction of SO₂ with the Surface of a Water Nanodroplet. Journal of the American Chemical Society, 2017, 139, 17168-17174.	6.6	46
77	Mechanistic Insights into Fast Charging and Discharging of the Sodium Metal Battery Anode: A Comparison with Lithium. Journal of the American Chemical Society, 2021, 143, 13929-13936.	6.6	46
78	The Formation of a Surprisingly Stable HO2âˆ'H2SO4Complex. Journal of the American Chemical Society, 2001, 123, 10387-10388.	6.6	45
79	Photodissociation Mechanisms of Major Mercury(II) Species in the Atmospheric Chemical Cycle of Mercury. Angewandte Chemie - International Edition, 2020, 59, 7605-7610.	7.2	45
80	Identifying the Molecular Origin of Global Warming. Journal of Physical Chemistry A, 2009, 113, 12694-12699.	1.1	44
81	Spontaneous Formation of One-Dimensional Hydrogen Gas Hydrate in Carbon Nanotubes. Journal of the American Chemical Society, 2014, 136, 10661-10668.	6.6	44
82	Pressure dependence and metastable state formation in the photolysis of dichlorine monoxide (Cl2O). Journal of Chemical Physics, 1996, 104, 2857-2868.	1.2	43
83	An Investigation of the Value of Using Concept Maps in General Chemistry. Journal of Chemical Education, 2001, 78, 1111.	1.1	43
84	The Gas-Phase Decomposition of CF₃OH with Water: A Radical-Catalyzed Mechanism. Journal of Physical Chemistry A, 2009, 113, 5333-5337.	1.1	43
85	Carboxylic Acid Catalyzed Hydration of Acetaldehyde. Journal of Physical Chemistry A, 2015, 119, 4581-4588.	1.1	43
86	TiO2 Photocatalytic Degradation of Dichloromethane:â€‰ An FTIR and Solid-State NMR Study. Journal of Physical Chemistry B, 2004, 108, 5640-5646.	1.2	42
87	Communication: Spectroscopic consequences of proton delocalization in OCHCO+. Journal of Chemical Physics, 2015, 143, 071102.	1.2	42
88	Evidence of low-density and high-density liquid phases and isochore end point for water confined to carbon nanotube. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4066-4071.	3.3	42
89	Photochemistry of SO₂ at the Airâ€"Water Interface: A Source of OH and HOSO Radicals. Journal of the American Chemical Society, 2018, 140, 12341-12344.	6.6	42
90	Single Atomâ€Modified Hybrid Transition Metal Carbides as Efficient Hydrogen Evolution Reaction Catalysts. Advanced Functional Materials, 2021, 31, 2104285.	7.8	42

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91	A spectroscopic case for SPSi detection: The third-row in a single molecule. Journal of Chemical Physics, 2016, 145, 124311.	1.2	41
92	Dimethylamine Addition to Formaldehyde Catalyzed by a Single Water Molecule: A Facile Route for Atmospheric Carbinolamine Formation and Potential Promoter of Aerosol Growth. Journal of Physical Chemistry A, 2016, 120, 1358-1368.	1.1	41
93	Gasâ€Phase Generation and Decomposition of a Sulfinylnitrene into the Iminyl Radical OSN. Angewandte Chemie - International Edition, 2016, 55, 1507-1510.	7.2	40
94	Gas-Phase Photolysis of Hg(I) Radical Species: A New Atmospheric Mercury Reduction Process. Journal of the American Chemical Society, 2019, 141, 8698-8702.	6.6	40
95	Criegee intermediate-hydrogen sulfide chemistry at the air/water interface. Chemical Science, 2017, 8, 5385-5391.	3.7	39
96	Parent Thioketene Sâ€Oxide H₂CCSO: Gasâ€Phase Generation, Structure, and Bonding Analysis. Chemistry - A European Journal, 2017, 23, 16566-16573.	1.7	39
97	A New Mechanism of Acid Rain Generation from HOSO at the Airâ€"Water Interface. Journal of the American Chemical Society, 2019, 141, 16564-16568.	6.6	39
98	A gas-to-particle conversion mechanism helps to explain atmospheric particle formation through clustering of iodine oxides. Nature Communications, 2020, 11, 4521.	5.8	39
99	Dissociation Pathways of Peroxyacetyl Nitrate (PAN). Journal of Physical Chemistry A, 1999, 103, 11451-11459.	1.1	38
100	The gas and solution phase acidities of HNO, HOONO, HONO, and HONO2. International Journal of Mass Spectrometry, 2003, 227, 421-438.	0.7	38
101	Controlling states of water droplets on nanostructured surfaces by design. Nanoscale, 2017, 9, 18240-18245.	2.8	38
102	Interfaces Select Specific Stereochemical Conformations: The Isomerization of Glyoxal at the Liquid Water Interface. Journal of the American Chemical Society, 2017, 139, 27-30.	6.6	38
103	Atmospheric Spectroscopy and Photochemistry at Environmental Water Interfaces. Annual Review of Physical Chemistry, 2019, 70, 45-69.	4.8	38
104	Photoinduced Oxidation Reactions at the Airâ€"Water Interface. Journal of the American Chemical Society, 2020, 142, 16140-16155.	6.6	38
105	Reaction pathways for gas-phase hydrolysis of formyl compounds HXCO (X = H, F, and Cl). Journal of the American Chemical Society, 1993, 115, 3746-3751.	6.6	37
106	Unimolecular Decomposition Pathways of Dimethyl Ether:â€‰ An ab Initio Study. Journal of Physical Chemistry A, 1998, 102, 236-241.	1.1	36
107	Crystal structure and encapsulation dynamics of ice II-structured neon hydrate. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10456-10461.	3.3	36
108	On the Detectability of the HSS, HSO, and HOS Radicals in the Interstellar Medium. Astrophysical Journal, 2017, 835, 243.	1.6	36

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109	Unraveling a New Chemical Mechanism of Missing Sulfate Formation in Aerosol Haze: Gaseous NO₂ with Aqueous HSO₃^{â€“}/SO₃^{2â€“}. Journal of the American Chemical Society, 2019, 141, 19312-19320.	6.6	36
110	High levelab initiostudies on the excited states of HOCO radical. Journal of Chemical Physics, 2000, 113, 7963-7970.	1.2	35
111	Ab Initio Study of Hydrogen Migration in 1-Alkylperoxy Radicals. Journal of Physical Chemistry A, 2010, 114, 11492-11505.	1.1	34
112	Hydrogen bonding and orientation effects on the accommodation of methylamine at the air-water interface. Journal of Chemical Physics, 2016, 144, 214701.	1.2	34
113	Simplest <i>N</i>-Sulfonylamine HNSO₂. Journal of the American Chemical Society, 2016, 138, 11509-11512.	6.6	34
114	Ab Initio Study of the Structure, Binding Energy, and Vibrations of the HOCl-H2O Complex. The Journal of Physical Chemistry, 1995, 99, 1919-1922.	2.9	33
115	Water Complexation as a Means of Stabilizing the Metastable HO3Radical. Journal of the American Chemical Society, 1999, 121, 8592-8596.	6.6	33
116	Surface Electrochemical Stability and Strainâ€Tunable Lithium Storage of Highly Flexible 2D Transition Metal Carbides. Advanced Functional Materials, 2018, 28, 1804867.	7.8	33
117	Direct observation of 2-dimensional ices on different surfaces near room temperature without confinement. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16723-16728.	3.3	33
118	Reactivity Trends within Alkoxy Radical Reactions Responsible for Chain Branching. Journal of the American Chemical Society, 2011, 133, 18208-18219.	6.6	32
119	A Computational Study Investigating the Energetics and Kinetics of the HNCO + (CH₃)₂NH Reaction Catalyzed by a Single Water Molecule. Journal of Physical Chemistry A, 2017, 121, 8465-8473.	1.1	32
120	Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO ₃. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24966-24971.	3.3	32
121	Ground and electronically excited states of methyl hydroperoxide: Comparison with hydrogen peroxide. Journal of Chemical Physics, 2006, 125, 104301.	1.2	31
122	Elemental sulfur aerosol-forming mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 864-869.	3.3	31
123	Molecular structure, vibrational frequencies, and energetics of the HOCO+ ion. Journal of Chemical Physics, 1997, 107, 9039-9045.	1.2	30
124	High levelab initiomolecular orbital theory study of the structure, vibrational spectrum, stability, and low-lying excited states of HOONO. Journal of Chemical Physics, 2000, 113, 7976-7981.	1.2	30
125	Accurateab initiostudy of the energetics of phosphorus nitride: Heat of formation, ionization potential, and electron affinity. Journal of Chemical Physics, 2003, 118, 8290-8295.	1.2	30
126	Temperature-Dependent Rate Coefficients for the Reaction of CH2OO with Hydrogen Sulfide. Journal of Physical Chemistry A, 2017, 121, 938-945.	1.1	30

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127	Mechanistic Insight into the Reaction of Organic Acids with SO₃ at the Airâ€"Water Interface. Angewandte Chemie - International Edition, 2019, 58, 8351-8355.	7.2	30
128	Two-dimensional semiconducting Lu₂CT₂(T = F, OH) MXene with low work function and high carrier mobility. Nanoscale, 2020, 12, 3795-3802.	2.8	30
129	Structure and Vibrational Spectra of Chlorofluorocarbon Substitutes:â€‰ An Experimental and ab Initio Study of Fluorinated Ethers CHF2OCF3 (E125), CHF2OCHF2 (E134), and CH3OCF3 (E143A). Journal of Physical Chemistry A, 1998, 102, 1854-1864.	1.1	29
130	Complexes of Hydroperoxyl Radical with Glyoxal, Methylglyoxal, Methylvinyl Ketone, Acrolein, and Methacrolein:â€‰ Possible New Sinks for HO2 in the Atmosphere?. Journal of Physical Chemistry A, 2003, 107, 2492-2496.	1.1	29
131	High-level ab initio studies of the structure, vibrational spectra, and energetics of S3. Journal of Chemical Physics, 2005, 123, 054302.	1.2	29
132	Complete active space self-consistent field and multireference configuration interaction studies of the differences between the low-lying excited states of HO2 and HO2â€"H2O. Journal of Chemical Physics, 1999, 110, 9017-9019.	1.2	28
133	The atmospheric oxidation of CH₃OOH by the OH radical: the effect of water vapor. Physical Chemistry Chemical Physics, 2017, 19, 12331-12342.	1.3	28
134	Mechanistic Quantification of Thermodynamic Stability and Mechanical Strength for Two-Dimensional Transition-Metal Carbides. Journal of Physical Chemistry C, 2018, 122, 4710-4722.	1.5	28
135	Revealing the Intrinsic Atomic Structure and Chemistry of Amorphous LiO₂-Containing Products in Liâ€"O₂ Batteries Using Cryogenic Electron Microscopy. Journal of the American Chemical Society, 2022, 144, 2129-2136.	6.6	28
136	A CASSCFâ€"MRCI study on the low-lying excited states of CH3OCl. Journal of Chemical Physics, 1999, 111, 8384-8388.	1.2	27
137	A molecular perspective for global modeling of upper atmospheric NH ₃ from freezing clouds. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6147-6152.	3.3	27
138	Triplet state promoted reaction of SO₂ with H₂O by competition between proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) processes. Physical Chemistry Chemical Physics, 2019, 21, 9779-9784.	1.3	27
139	First-Principles Molecular Dynamics Simulations of the Spontaneous Freezing Transition of 2D Water in a Nanoslit. Journal of the American Chemical Society, 2021, 143, 8177-8183.	6.6	27
140	High level ab initio molecular orbital study of the structures and vibrational spectra of CHBr+ and CBr+. Journal of Chemical Physics, 1998, 109, 134-138.	1.2	26
141	The Impact of Continuous Instructional Development on Graduate and Undergraduate Students. Journal of Chemical Education, 1999, 76, 114.	1.1	26
142	Heteroatom Tuning of Bimolecular Criegee Reactions and Its Implications. Angewandte Chemie - International Edition, 2016, 55, 13432-13435.	7.2	26
143	Elucidating the molecular mechanisms of Criegee-amine chemistry in the gas phase andÂaqueous surface environments. Chemical Science, 2019, 10, 743-751.	3.7	26
144	Hydration, Solvation, and Isomerization of Methylglyoxal at the Air/Water Interface: New Mechanistic Pathways. Journal of the American Chemical Society, 2020, 142, 5574-5582.	6.6	26

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145	Structures, Vibrational Spectra, and Relative Energetics of HBrO3 Isomers. Journal of Physical Chemistry A, 1998, 102, 2072-2079.	1.1	25
146	Anab initiostudy of the competing reaction channels in the reaction of HOCO radicals with NO and O2. Journal of Chemical Physics, 2004, 120, 5073-5080.	1.2	25
147	Identifying Cytosine-Specific Isomers via High-Accuracy Single Photon Ionization. Journal of the American Chemical Society, 2016, 138, 16596-16599.	6.6	25
148	Ion pair particles at the airâ€“water interface. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12401-12406.	3.3	25
149	Is AlOH the Astrochemical Reservoir Molecule of AlO?: Insights from Excited Electronic States. Astrophysical Journal, 2018, 863, 139.	1.6	25
150	Spectroscopic investigation of [Al,N,C,O] refractory molecules. Journal of Chemical Physics, 2019, 151, 244303.	1.2	25
151	Water transport through subnanopores in the ultimate size limit: Mechanism from molecular dynamics. Nano Research, 2019, 12, 587-592.	5.8	25
152	Turning a Superhydrophilic Surface Weakly Hydrophilic: Topological Wetting States. Journal of the American Chemical Society, 2020, 142, 18491-18502.	6.6	25
153	Dissociation dynamics of FC(O)O and ClC(O)O radicals. Chemical Physics, 1988, 127, 73-79.	0.9	24
154	Theoretical Study of the Thermal Decomposition Pathways of 2-H Heptafluoropropane. Journal of Physical Chemistry A, 2002, 106, 3106-3113.	1.1	24
155	Anab initiostudy of the pathways for the reaction between CH3O2 and BrO radicals. Journal of Chemical Physics, 2003, 118, 1779-1793.	1.2	24
156	ClClO2 Is the Most Stable Isomer of Cl2O2. Accurate Coupled Cluster Energetics and Electronic Spectra of Cl2O2 Isomers. Journal of Physical Chemistry A, 2008, 112, 9623-9627.	1.1	24
157	Thermodynamic Properties of the Isomers of [HNOS], [HNO₂S], and [HNOS₂] and the Role of the Central Sulfur. Chemistry - A European Journal, 2014, 20, 10231-10235.	1.7	24
158	The Role of Catalysis in Alkanediol Decomposition: Implications for General Detection of Alkanediols and Their Formation in the Atmosphere. Journal of Physical Chemistry A, 2015, 119, 9821-9833.	1.1	24
159	The Stability of Î±â€Hydroperoxyalkyl Radicals. Chemistry - A European Journal, 2016, 22, 18092-18100.	1.7	24
160	Single-Molecule Catalysis Revealed: Elucidating the Mechanistic Framework for the Formation and Growth of Atmospheric Iodine Oxide Aerosols in Gas-Phase and Aqueous Surface Environments. Journal of the American Chemical Society, 2018, 140, 14704-14716.	6.6	24
161	Evidence of the Elusive Gold-Induced Non-classical Hydrogen Bonding in Aqueous Environments. Journal of the American Chemical Society, 2020, 142, 6001-6006.	6.6	24
162	Theoretical spectroscopic investigations of HNSq and HSNq (q = 0, +1, âˆ'1) in the gas phase. Journal of Chemical Physics, 2014, 140, 244309.	1.2	23

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