C Franklin Goldsmith

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3454524/publications.pdf

Version: 2024-02-01

67 papers	2,407 citations	201674 27 h-index	214800 47 g-index
68 all docs	68 docs citations	68 times ranked	1589 citing authors

#	Article	IF	Citations
1	Non-Idealities in Lab-Scale Kinetic Testing: A Theoretical Study of a Modular Temkin Reactor. Catalysts, 2022, 12, 349.	3.5	9
2	Comparison of flame inception behavior of liquid nitromethane in inert and air environments. Combustion and Flame, 2022, 241, 112101.	5.2	3
3	Laminar flame speeds and ignition delay times for isopropyl nitrate and propane blends. Combustion and Flame, 2022, 242, 112187.	5.2	6
4	Shock tube study of the pyrolysis kinetics of Di- and trimethoxy methane. Combustion and Flame, 2022, 242, 112186.	5.2	3
5	Low-temperature oxidation of diethyl ether: Reactions of hot radicals across coupled potential energy surfaces. Proceedings of the Combustion Institute, 2021, 38, 671-679.	3.9	16
6	A statistical model for the product energy distribution in reactions leading to prompt dissociation. Proceedings of the Combustion Institute, 2021, 38, 507-514.	3.9	6
7	Ring opening in cycloheptane and dissociation of 1-heptene at high temperatures. Proceedings of the Combustion Institute, 2021, 38, 929-937.	3.9	3
8	Laser schlieren study of the thermal decomposition of 2-ethylhexyl-nitrate. Proceedings of the Combustion Institute, 2021, 38, 997-1005.	3.9	12
9	The impact of NO_x addition on the ignition behaviour of n-pentane. Reaction Chemistry and Engineering, 2021, 6, 2191-2203.	3.7	7
10	Transition-metal-mediated reduction and reversible double-cyclization of cyanuric triazide to an asymmetric bitetrazolate involving cleavage of the six-membered aromatic ring. Chemical Science, 2021, 12, 2268-2275.	7.4	3
11	A continuous flow liquid propellant strand burner for high pressure monopropellant and bipropellant combustion studies. Review of Scientific Instruments, 2021, 92, 025106.	1.3	3
12	Microkinetic Modeling of the CO₂ Desorption from Supported Multifaceted Ni Catalysts. Journal of Physical Chemistry C, 2021, 125, 2984-3000.	3.1	20
13	Combustion chemistry in the twenty-first century: Developing theory-informed chemical kinetics models. Progress in Energy and Combustion Science, 2021, 83, 100886.	31.2	89
14	Reaction Mechanism Generator v3.0: Advances in Automatic Mechanism Generation. Journal of Chemical Information and Modeling, 2021, 61, 2686-2696.	5.4	116
15	Automated Mechanism Generation Using Linear Scaling Relationships and Sensitivity Analyses Applied to Catalytic Partial Oxidation of Methane. ACS Catalysis, 2021, 11, 7114-7125.	11.2	20
16	Rate coefficients for 1,2-dimethyl-allylâ€¯+â€¯HO2/O2 and the implications for 2-methyl-2-butene combustion. Combustion and Flame, 2021, 230, 111433.	5.2	4
17	Quantifying the Impact of Parametric Uncertainty on Automatic Mechanism Generation for CO₂ Hydrogenation on Ni(111). Jacs Au, 2021, 1, 1656-1673.	7.9	30
18	Adsorbate Partition Functions via Phase Space Integration: Quantifying the Effect of Translational Anharmonicity on Thermodynamic Properties. Journal of Physical Chemistry C, 2021, 125, 20249-20260.	3.1	9

#	Article	IF	Citations
19	Diastereomers and Low-Temperature Oxidation. Journal of Physical Chemistry A, 2021, 125, 8064-8073.	2.5	11
20	Heterogeneity in susceptibility dictates the order of epidemic models. Journal of Theoretical Biology, 2021, 528, 110839.	1.7	14
21	Non-Boltzmann Effects in Chain Branching and Pathway Branching for Diethyl Ether Oxidation. Energy & Fuels, 2021, 35, 17890-17908.	5.1	16
22	Accelerating Variational Transition State Theory via Artificial Neural Networks. Journal of Physical Chemistry A, 2020, 124, 1038-1046.	2.5	14
23	Development of a Microkinetic Model for the CO2 Methanation with an Automated Reaction Mechanism Generator. Computer Aided Chemical Engineering, 2020, 48, 529-534.	0.5	7
24	Thermal Stability of Bis-Tetrazole and Bis-Triazole Derivatives with Long Catenated Nitrogen Chains: Quantitative Insights from High-Level Quantum Chemical Calculations. Journal of Physical Chemistry A, 2020, 124, 7665-7677.	2.5	15
25	Thermal dissociation of alkyl nitrites and recombination of alkyl radicals. Proceedings of the Combustion Institute, 2019, 37, 703-710.	3.9	9
26	A modular, multi-diagnostic, automated shock tube for gas-phase chemistry. Review of Scientific Instruments, 2019, 90, 064104.	1.3	6
27	Accurate Thermochemistry of Novel Energetic Fused Tricyclic 1,2,3,4-Tetrazine Nitro Derivatives from Local Coupled Cluster Methods. Journal of Physical Chemistry A, 2019, 123, 9818-9827.	2.5	20
28	Computer-Generated Kinetics for Coupled Heterogeneous/Homogeneous Systems: A Case Study in Catalytic Combustion of Methane on Platinum. Industrial & Engineering Chemistry Research, 2019, 58, 17682-17691.	3.7	26
29	Decomposition kinetics for HONO and HNO₂. Reaction Chemistry and Engineering, 2019, 4, 323-333.	3.7	52
30	Shock Tube Laser Schlieren Study of the Pyrolysis of Isopropyl Nitrate. Journal of Physical Chemistry A, 2019, 123, 5866-5876.	2.5	11
31	Accurate Prediction of Bond Dissociation Energies and Barrier Heights for High-Energy Caged Nitro and Nitroamino Compounds Using a Coupled Cluster Theory. Journal of Physical Chemistry A, 2019, 123, 4883-4890.	2.5	34
32	Predictive kinetics for the thermal decomposition of RDX. Proceedings of the Combustion Institute, 2019, 37, 3167-3173.	3.9	34
33	On the relative importance of HONO versus HNO2 in low-temperature combustion. Proceedings of the Combustion Institute, 2019, 37, 695-702.	3.9	20
34	Direct measurements of channel specific rate constants in OHâ€¯+â€¯C3H8 illuminates prompt dissociations of propyl radicals. Proceedings of the Combustion Institute, 2019, 37, 231-238.	3.9	16
35	A computational investigation into the combustion byproducts of a liquid monopropellant. Proceedings of the Combustion Institute, 2019, 37, 5671-5677.	3.9	6
36	A computational investigation into the kinetics of NO + CH2CCH and its effect on NO reduction. Proceedings of the Combustion Institute, 2019, 37, 687-694.	3.9	6

#	Article	IF	Citations
37	High temperature pyrolysis of 2-methyl furan. Physical Chemistry Chemical Physics, 2018, 20, 10826-10837.	2.8	17
38	Toward reliable characterization of energetic materials: interplay of theory and thermal analysis in the study of the thermal stability of tetranitroacetimidic acid (TNAA). Physical Chemistry Chemical Physics, 2018, 20, 29285-29298.	2.8	24
39	The impact of roaming radicals on the combustion properties of transportation fuels. Combustion and Flame, 2018, 194, 387-395.	5.2	16
40	A combined photoionization time-of-flight mass spectrometry and laser absorption spectrometry flash photolysis apparatus for simultaneous determination of reaction rates and product branching. Review of Scientific Instruments, 2018, 89, 074102.	1.3	11
41	Chemical Kinetics of Hydrogen Atom Abstraction from Allylic Sites by ³O₂; Implications for Combustion Modeling and Simulation. Journal of Physical Chemistry A, 2017, 121, 1890-1899.	2.5	44
42	Automatic Generation of Microkinetic Mechanisms for Heterogeneous Catalysis. Journal of Physical Chemistry C, 2017, 121, 9970-9981.	3.1	80
43	An Experimental and Theoretical Study of the Thermal Decomposition of C₄H₆ Isomers. Journal of Physical Chemistry A, 2017, 121, 3827-3850.	2.5	20
44	A Theoretical and Computational Analysis of the Methyl-Vinyl + O2 Reaction and Its Effects on Propene Combustion. Journal of Physical Chemistry A, 2017, 121, 9173-9184.	2.5	23
45	Rate coefficients for fuel + NO2: Predictive kinetics for HONO and HNO2 formation. Proceedings of the Combustion Institute, 2017, 36, 617-626.	3.9	64
46	Ramifications of including non-equilibrium effects for HCO in flame chemistry. Proceedings of the Combustion Institute, 2017, 36, 525-532.	3.9	36
47	Experimental and Kinetic Modeling Study of C₂H₂ Oxidation at High Pressure. International Journal of Chemical Kinetics, 2016, 48, 724-738.	1.6	67
48	Weakly Bound Free Radicals in Combustion: â€œPromptâ€•Dissociation of Formyl Radicals and Its Effect on Laminar Flame Speeds. Journal of Physical Chemistry Letters, 2016, 7, 85-89.	4.6	63
49	Comment on â€œWhen Rate Constants Are Not Enoughâ€• Journal of Physical Chemistry A, 2016, 120, 306-312.	2.5	30
50	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7766-7779.	2.5	88
51	Towards a quantitative understanding of the role of non-Boltzmann reactant distributions in low temperature oxidation. Proceedings of the Combustion Institute, 2015, 35, 205-213.	3.9	48
52	Multiscale Informatics for Low-Temperature Propane Oxidation: Further Complexities in Studies of Complex Reactions. Journal of Physical Chemistry A, 2015, 119, 7095-7115.	2.5	37
53	New Insights into Low-Temperature Oxidation of Propane from Synchrotron Photoionization Mass Spectrometry and Multiscale Informatics Modeling. Journal of Physical Chemistry A, 2015, 119, 7116-7129.	2.5	32
54	Understanding low-temperature first-stage ignition delay: Propane. Combustion and Flame, 2015, 162, 3658-3673.	5.2	122

#	Article	IF	Citations
55	Effect of non-thermal product energy distributions on ketohydroperoxide decomposition kinetics. Proceedings of the Combustion Institute, 2015, 35, 283-290.	3.9	58
56	A shock tube laser schlieren study of methyl acetate dissociation in the fall-off regime. Physical Chemistry Chemical Physics, 2014, 16, 7241.	2.8	13
57	Catalytic partial oxidation of methane on platinum investigated by spatial reactor profiles, spatially resolved spectroscopy, and microkinetic modeling. Journal of Catalysis, 2013, 297, 1-16.	6.2	82
58	Uncertainty propagation in the derivation of phenomenological rate coefficients from theory: A case study of n-propyl radical oxidation. Proceedings of the Combustion Institute, 2013, 34, 177-185.	3.9	64
59	Propargyl + O₂ Reaction in Helium Droplets: Entrance Channel Barrier or Not?. Journal of Physical Chemistry A, 2013, 117, 13626-13635.	2.5	39
60	Role of O₂ + QOOH in Low-Temperature Ignition of Propane. 1. Temperature and Pressure Dependent Rate Coefficients. Journal of Physical Chemistry A, 2012, 116, 3325-3346.	2.5	223
61	Automatic estimation of pressure-dependent rate coefficients. Physical Chemistry Chemical Physics, 2012, 14, 1131-1155.	2.8	96
62	Database of Small Molecule Thermochemistry for Combustion. Journal of Physical Chemistry A, 2012, 116, 9033-9057.	2.5	178
63	Estimating the Thermochemistry of Adsorbates Based Upon Gas-Phase Properties. Topics in Catalysis, 2012, 55, 366-375.	2.8	19
64	Theoretical rate coefficients for allyl+HO2 and allyloxy decomposition. Proceedings of the Combustion Institute, 2011, 33, 273-282.	3.9	75
65	Decomposition and Vibrational Relaxation in CH₃I and Self-Reaction of CH₃ Radicals. Journal of Physical Chemistry A, 2009, 113, 8307-8317.	2.5	33
66	Pressure and Temperature Dependence of the Reaction of Vinyl Radical with Alkenes III: Measured Rates and Predicted Product Distributions for Vinyl + Butene. Journal of Physical Chemistry A, 2009, 113, 13357-13371.	2.5	9
67	Pressure and Temperature Dependence of the Reaction of Vinyl Radical with Ethyleneâ€. Journal of Physical Chemistry A, 2007, 111, 6843-6851.	2.5	20