Michael Frenklach

List of Publications by Year
in descending order

131 papers	12,734 citations	36203 51 h-index	23472 111 g-index
132 all docs	132 docs citations	132 times ranked	4536 citing authors

#	Article	IF	Citations
1	Mechanism of E-bridge formation by various PAH molecules: A theoretical study. Chemical Physics Letters, 2022, 799, 139637.	1.2	5
2	Why turquoise hydrogen will Be a game changer for the energy transition. International Journal of Hydrogen Energy, 2022, 47, 25831-25848.	3.8	50
3	Formation of phenanthrenyl radicals via the reaction of acenaphthyl with acetylene. Proceedings of the Combustion Institute, 2021, 38, 1441-1448.	2.4	12
4	Does a reduced model reproduce the uncertainty of the original full-size model?. Combustion and Flame, 2021, 226, 98-107.	2.8	4
5	Representing Model Discrepancy in Bound-to-Bound Data Collaboration. SIAM-ASA Journal on Uncertainty Quantification, 2021, 9, 231-259.	1.1	5
6	Transformation of an Embedded Five-Membered Ring in Polycyclic Aromatic Hydrocarbons via the Hydrogen-Abstractionâ€“Acetylene-Addition Mechanism: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 3341-3354.	1.1	10
7	On the Mechanism of Soot Nucleation. III. The Fate and Facility of the E-Bridge. Journal of Physical Chemistry A, 2021, 125, 6789-6795.	1.1	6
8	Quantifying uncertainty in kinetic simulation of engine autoignition. Combustion and Flame, 2020, 216, 174-184.	2.8	17
9	On the mechanism of soot nucleation. II. E-bridge formation at the PAH bay. Physical Chemistry Chemical Physics, 2020, 22, 17196-17204.	1.3	14
10	On the mechanism of soot nucleation. Physical Chemistry Chemical Physics, 2020, 22, 5314-5331.	1.3	136
11	Rate constants for the formation of the vinylidene bridge bond between naphthalene and acenaphthalene: A theoretical study. AIP Conference Proceedings, 2020, , .	0.3	0
12	Aceanthracene-anthracene dimerization with the formation of an E-bridge bond. AIP Conference Proceedings, 2020, , .	0.3	0
13	On the low-temperature limit of HACA. Proceedings of the Combustion Institute, 2019, 37, 969-976.	2.4	62
14	New form for reduced modeling of soot oxidation: Accounting for multi-site kinetics and surface reactivity. Combustion and Flame, 2019, 201, 148-159.	2.8	22
15	Investigation of Dataset Construction Parameters and their Impact on Reaction Model Optimization using PrIMe. , 2018, , .		1
16	Detailed, sterically-resolved modeling of soot oxidation: Role of O atoms, interplay with particle nanostructure, and emergence of inner particle burning. Combustion and Flame, 2018, 188, 284-306.	2.8	81
17	Diagnostics of Data-Driven Models: Uncertainty Quantification of PM7 Semi-Empirical Quantum Chemical Method. Scientific Reports, 2018, 8, 13248.	1.6	8
18	Application of Bound-to-Bound Data Collaboration approach for development and uncertainty quantification of a reduced char combustion model. Fuel, 2018, 232, 769-779.	3.4	14

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19	Consistency Analysis for Massively Inconsistent Datasets in Bound-to-Bound Data Collaboration. SIAM-ASA Journal on Uncertainty Quantification, 2018, 6, 429-456.	1.1	10
20	Consistent Syngas Chemical Mechanism from Collaborative Data Processing. , 2017, , .		0
21	Development of an Uncertainty Quantification Predictive Chemical Reaction Model for Syngas Combustion. Energy & Fuels, 2017, 31, 2274-2297.	2.5	28
22	Rate constants for H abstraction from benzo(a)pyrene and chrysene: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 25401-25413.	1.3	37
23	A mechanistic study of the influence of graphene curvature on the rate of high-temperature oxidation by molecular oxygen. Carbon, 2016, 101, 203-212.	5.4	38
24	Quantum Monte Carlo Study of the Reactions of CH with Acrolein: Major and Minor Channels. Journal of Physical Chemistry A, 2016, 120, 3602-3612.	1.1	21
25	Comparison of Statistical and Deterministic Frameworks of Uncertainty Quantification. SIAM-ASA Journal on Uncertainty Quantification, 2016, 4, 875-901.	1.1	33
26	Consistent Chemical Mechanism from Collaborative Data Processing. , 2016, , .		1
27	Reply to â€œComment on â€˜When Rate Constants Are Not Enoughâ€™â€•. Journal of Physical Chemistry A, 2016, 120, 313-317.	1.1	5
28	Effect of Reaction Kinetics on Graphene-Edge Morphology and Composition. Zeitschrift Fur Physikalische Chemie, 2015, 229, 597-614.	1.4	22
29	Rate coefficients and product branching ratios for the oxidation of phenyl and naphthyl radicals: A theoretical RRKM-ME study. Proceedings of the Combustion Institute, 2015, 35, 1861-1869.	2.4	34
30	Oxidation of Graphene-Edge Six- and Five-Member Rings by Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7528-7547.	1.1	46
31	A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. Journal of Physical Chemistry A, 2015, 119, 4214-4223.	1.1	28
32	When Rate Constants Are Not Enough. Journal of Physical Chemistry A, 2015, 119, 7451-7461.	1.1	18
33	Integrated data-model analysis facilitated by an Instrumental Model. Proceedings of the Combustion Institute, 2015, 35, 597-605.	2.4	14
34	Interval Prediction of Molecular Properties in Parametrized Quantum Chemistry. Physical Review Letters, 2014, 112, 253003.	2.9	12
35	Pathways to Soot Oxidation: Reaction of OH with Phenanthrene Radicals. Journal of Physical Chemistry A, 2014, 118, 8606-8613.	1.1	43
36	Thermal decomposition of graphene armchair oxyradicals. Proceedings of the Combustion Institute, 2013, 34, 1759-1766.	2.4	17

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37	Process informatics tools for predictive modeling: Hydrogen combustion. International Journal of Chemical Kinetics, 2012, 44, 101-116.	1.0	44
38	Thermal Decomposition of Pentacene Oxyradicals. Journal of Physical Chemistry A, 2011, 115, 14184-14190.	1.1	31
39	Patterns of local aromaticity in graphene oxyradicals. Journal of Materials Chemistry, 2011, 21, 3404.	6.7	13
40	Bay-capping reactions: Kinetics and influence on graphene-edge growth. Proceedings of the Combustion Institute, 2011, 33, 685-692.	2.4	31
41	Optimization of combustion kinetic models on a feasible set. Proceedings of the Combustion Institute, 2011, 33, 509-516.	2.4	67
42	Uncertainty quantification: Making predictions of complex reaction systems reliable. Chemical Physics Letters, 2010, 499, 1-8.	1.2	45
43	Substrate-free microwave synthesis of graphene: experimental conditions and hydrocarbon precursors. New Journal of Physics, 2010, 12, 125013.	1.2	86
44	Local Electronic Structure and Stability of Pentacene Oxyradicals. Journal of Physical Chemistry C, 2010, 114, 5429-5437.	1.5	20
45	Detailed Kinetic Monte Carlo Simulations of Graphene-Edge Growth. Journal of Physical Chemistry A, 2010, 114, 689-703.	1.1	120
46	Embedded-ring migration on graphene zigzag edge. Proceedings of the Combustion Institute, 2009, 32, 577-583.	2.4	33
47	Graphene Layer Growth Chemistry:â€‰ Five- and Six-Member Ring Flip Reaction. Journal of Physical Chemistry A, 2008, 112, 2125-2130.	1.1	35
48	Sensitivity Analysis of Uncertainty in Model Prediction. Journal of Physical Chemistry A, 2008, 112, 2579-2588.	1.1	69
49	Chapter 6 Optimization of Reaction Models with Solution Mapping. Comprehensive Chemical Kinetics, 2007, 42, 243-291.	2.3	23
50	A CSP and tabulation-based adaptive chemistry model. Combustion Theory and Modelling, 2007, 11, 73-102.	1.0	35
51	Graphene layer growth: Collision of migrating five-member rings. Proceedings of the Combustion Institute, 2007, 31, 539-546.	2.4	55
52	Transforming data into knowledgeâ€”Process Informatics for combustion chemistry. Proceedings of the Combustion Institute, 2007, 31, 125-140.	2.4	150
53	A system analysis approach for atmospheric observations and models: Mesospheric HOx dilemma. Journal of Geophysical Research, 2006, 111, .	3.3	21
54	Model Discrimination Using Data Collaborationâ€. Journal of Physical Chemistry A, 2006, 110, 6803-6813.	1.1	55

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55	Quantum Monte Carlo study of small hydrocarbon atomization energies. Molecular Physics, 2006, 104, 467-475.	0.8	0
56	Numerical approaches for collaborative data processing. Optimization and Engineering, 2006, 7, 459-478.	1.3	47
57	Migration mechanism of aromatic-edge growth. Proceedings of the Combustion Institute, 2005, 30, 1389-1396.	2.4	57
58	Quantum monte carlo study of heats of formation and bond dissociation energies of small hydrocarbons. International Journal of Chemical Kinetics, 2005, 37, 583-592.	1.0	11
59	Detailed kinetic modeling of soot aggregate formation in laminar premixed flames. Combustion and Flame, 2005, 140, 130-145.	2.8	98
60	Collaborative data processing in developing predictive models of complex reaction systems. International Journal of Chemical Kinetics, 2004, 36, 57-66.	1.0	117
61	Consistency of a Reaction Dataset. Journal of Physical Chemistry A, 2004, 108, 9573-9583.	1.1	79
62	Computational economy improvements in PRISM. International Journal of Chemical Kinetics, 2003, 35, 438-452.	1.0	32
63	Experimental and modeling study of shock-tube oxidation of acetylene. International Journal of Chemical Kinetics, 2003, 35, 391-414.	1.0	54
64	Prediction uncertainty from models and data. , 2002, , .		15
65	Reaction mechanism of soot formation in flames. Physical Chemistry Chemical Physics, 2002, 4, 2028-2037.	1.3	1,260
66	Nucleation of soot: Molecular dynamics simulations of pyrene dimerization. Proceedings of the Combustion Institute, 2002, 29, 2307-2314.	2.4	189
67	Method of moments with interpolative closure. Chemical Engineering Science, 2002, 57, 2229-2239.	1.9	328
68	A quantum Monte Carlo study of energy differences in C4H3 and C4H5 isomers. International Journal of Chemical Kinetics, 2001, 33, 808-820.	1.0	18
69	Kinetic modeling of soot formation with detailed chemistry and physics: laminar premixed flames of C2 hydrocarbons. Combustion and Flame, 2000, 121, 122-136.	2.8	1,035
70	Comment on â€œRate Constants for CH3 + O2 â† CH3O + O at High Temperature and Evidence for H2CO + O2 â† HCO + HO2â€•and â€œRate Coefficient Measurements of the Reaction CH3 + O2 = CH3O + Oâ€• Journal of Physical Chemistry A, 2000, 104, 9797-9799.	1.1	4
71	Hydrogen Migration in the Phenylethen-2-yl Radical. Journal of Physical Chemistry A, 1999, 103, 7127-7135.	1.1	48
72	PRISM: Piecewise Reusable Implementation of Solution Mapping. An Economical Strategy for Chemical Kinetics. Israel Journal of Chemistry, 1999, 39, 97-106.	1.0	95

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73	Dynamic Modeling of Soot Particle Coagulation and Aggregation: Implementation With the Method of Moments and Application to High-Pressure Laminar Premixed Flames. Combustion and Flame, 1998, 114, 484-501.	2.8	241
74	Hydrogen migration in polyaromatic growth. Proceedings of the Combustion Institute, 1998, 27, 1655-1661.	0.3	51
75	Detailed kinetic modeling of soot formation in ethylene/air mixtures reacting in a perfectly stirred reactor. Proceedings of the Combustion Institute, 1998, 27, 1573-1580.	0.3	24
76	Determination of Rate Coefficients for Reactions of Formaldehyde Pyrolysis and Oxidation in the Gas Phase. Journal of Physical Chemistry A, 1998, 102, 5196-5205.	1.1	64
77	Kinetic Monte Carlo Simulation of Diamond Film Growth with the Inclusion of Surface Migration. Materials Research Society Symposia Proceedings, 1998, 527, 383.	0.1	4
78	Surface Migration in Diamond Growth. Journal of Physical Chemistry B, 1997, 101, 3025-3036.	1.2	76
79	A detailed kinetic modeling study of aromatics formation in laminar premixed acetylene and ethylene flames. Combustion and Flame, 1997, 110, 173-221.	2.8	1,070
80	Silicon Particle Formation in Pyrolysis of Silane and Disilane. Israel Journal of Chemistry, 1996, 36, 293-303.	1.0	36
81	On surface growth mechanism of soot particles. Proceedings of the Combustion Institute, 1996, 26, 2285-2293.	0.3	90
82	A One-Dimensional Stochastic Model of Diamond Growth. Materials Research Society Symposia Proceedings, 1995, 399, 83.	0.1	0
83	A Theoretical Study Of The Energetics And Vibrational Spectra Of Oxygenated (100) Diamond Surfaces. Materials Research Society Symposia Proceedings, 1995, 416, 281.	0.1	0
84	A post-processing method for feature sensitivity coefficients. International Journal of Chemical Kinetics, 1995, 27, 1135-1142.	1.0	3
85	Detailed modeling of soot formation in laminar premixed ethylene flames at a pressure of 10 bar. Combustion and Flame, 1995, 100, 111-120.	2.8	222
86	A theoretical analysis of a diamond (100)â€(2Ã—1) dimer bond. Journal of Chemical Physics, 1995, 102, 5486-5491.	1.2	37
87	Calculations of Rate Coefficients for the Chemically Activated Reactions of Acetylene with Vinylic and Aromatic Radicals. The Journal of Physical Chemistry, 1994, 98, 11465-11489.	2.9	301
88	Reduced mechanism of soot formationâ€"Applicationto natural gas-fueled diesel combustion. Proceedings of the Combustion Institute, 1994, 25, 941-948.	0.3	30
89	Transport properties of polycyclic aromatic hydrocarbons for flame modelingâ˜†. Combustion and Flame, 1994, 96, 163-170.	2.8	237
90	An atomistic model for stepped diamond growth. Nature, 1994, 372, 535-537.	13.7	50

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91	Chemical Reaction Mechanisms of Diamond Growth. Materials Research Society Symposia Proceedings, 1994, 339, 255.	0.1	3
92	Oxygen poisoning of diamond film growth. Applied Physics Letters, 1993, 63, 2641-2643.	1.5	11
93	Molecular dynamics with combined quantum and empirical potentials: C2H2 adsorption on Si(100). Journal of Chemical Physics, 1993, 99, 1356-1372.	1.2	93
94	Theoretical study of reaction between phenylvinyleum ion and acetylene. The Journal of Physical Chemistry, 1993, 97, 10364-10371.	2.9	8
95	Monte Carlo simulation of hydrogen reactions with the diamond surface. Physical Review B, 1992, 45, 9455-9458.	1.1	25
96	Cyclic deposition of diamond: Experimental testing of model predictions. Journal of Applied Physics, 1992, 72, 5926-5940.	1.1	16
97	Monte Carlo simulation of diamond growth by methyl and acetylene reactions. Journal of Chemical Physics, 1992, 97, 5794-5802.	1.2	71
98	Optimization and analysis of large chemical kinetic mechanisms using the solution mapping methodâ€"combustion of methane. Progress in Energy and Combustion Science, 1992, 18, 47-73.	15.8	369
99	Induced nucleation of diamond powder. Applied Physics Letters, 1991, 59, 546-548.	1.5	97
100	A New Mechanism for the Formation of Meteoritic Kerogen-Like Material. Science, 1991, 252, 109-112.	6.0	49
101	Detailed modeling of soot particle nucleation and growth. Proceedings of the Combustion Institute, 1991, 23, 1559-1566.	0.3	876
102	Detailed reduction of reaction mechanisms for flame modeling. Combustion and Flame, 1991, 87, 365-370.	2.8	158
103	Analysis of cyclic deposition of diamond. Journal of Applied Physics, 1991, 70, 7132-7136.	1.1	7
104	Soot formation in shock-tube pyrolysis and oxidation of vinylacetylene. AIP Conference Proceedings, 1990, , .	0.3	1
105	Kinetics of Titanium(IV) Chloride Oxidation. Journal of the American Ceramic Society, 1990, 73, 2158-2162.	1.9	124
106	Production of Polycyclic Aromatic Hydrocarbons in Chlorine Containing Environments*. Combustion Science and Technology, 1990, 74, 283-296.	1.2	69
107	Formation of silicon carbide particles behind shock waves. Applied Physics Letters, 1989, 54, 1430-1432.	1.5	21
108	The role of hydrogen in vapor deposition of diamond. Journal of Applied Physics, 1989, 65, 5142-5149.	1.1	193

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109	On the driving force of PAH production. Proceedings of the Combustion Institute, 1989, 22, 1075-1082.	0.3	44
110	Silicon carbide and the origin of interstellar carbon grains. Nature, 1989, 339, 196-198.	13.7	52
111	Effect of fuel structure on pathways to soot. Proceedings of the Combustion Institute, 1988, 21, 1067-1076.	0.3	92
112	Comment on the proposed role of spheroidal carbon clusters in soot formation. The Journal of Physical Chemistry, 1988, 92, 561-563.	2.9	95
113	Growth mechanism of vapor-deposited diamond. Journal of Materials Research, 1988, 3, 133-140.	1.2	369
114	Soot formation in binary hydrocarbon mixtures. Energy & Fuels, 1988, 2, 462-480.	2.5	94
115	Detailed Modeling of PAH Profiles in a Sooting Low-Pressure Acetylene Flame. Combustion Science and Technology, 1987, 51, 265-283.	1.2	388
116	Aerosol dynamics modeling using the method of moments. Journal of Colloid and Interface Science, 1987, 118, 252-261.	5.0	357
117	Soot formation in shock-tube oxidation of hydrocarbons. Proceedings of the Combustion Institute, 1985, 20, 871-878.	0.3	44
118	Detailed kinetic modeling of soot formation in shock-tube pyrolysis of acetylene. Proceedings of the Combustion Institute, 1985, 20, 887-901.	0.3	502
119	Dynamics of discrete distribution for Smoluchowski coagulation model. Journal of Colloid and Interface Science, 1985, 108, 237-242.	5.0	50
120	Computer modeling of infinite reaction sequences: A chemical lumping. Chemical Engineering Science, 1985, 40, 1843-1849.	1.9	63
121	Statistically rigorous parameter estimation in dynamic modeling using approximate empirical models. AICHE Journal, 1985, 31, 498-500.	1.8	29
122	DISCUSSION of the Bates-Watts paper, Multiresponse Estimation With Special Applications to First Order Kinetics. Journal of Research of the National Bureau of Standards (United States), 1985, 90, 438-439.	0.3	0
123	Some new ideas in the analysis of screening designs - Discussion. Journal of Research of the National Bureau of Standards (United States), 1985, 90, 501-502.	0.3	0
124	Shock-initiated ignition in methane-propane mixtures. Combustion and Flame, 1984, 56, 1-27.	2.8	111
125	Systematic optimization of a detailed kinetic model using a methane ignition example. Combustion and Flame, 1984, 58, 69-72.	2.8	92
126	Representation of multistage mechanisms in detailed computer modeling of polymerization kinetics. The Journal of Physical Chemistry, 1984, 88, 6263-6266.	2.9	14

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127	Sensitivity analysis and parameter estimation in dynamic modeling of chemical kinetics. International Journal of Chemical Kinetics, 1983, 15, 677-696.	1.0	90
128	Soot formation in shock-tube pyrolysis of acetylene, allene, and 1,3-butadieneâ˜†. Combustion and Flame, 1983, 54, 81-101.	2.8	170
129	Oxidation of cyanogen. II. The mechanism of the oxidation. International Journal of Chemical Kinetics, 1980, 12, 159-168.	1.0	30
130	The reaction between H2 and D2 in a shock tube: Study of the atomic vs molecular mechanism by atomic resonance absorption spectrometry. Journal of Chemical Physics, 1977, 67, 2803.	1.2	19
131	Cleavage of an aromatic ring and radical migration. Faraday Discussions, 0, , .	1.6	1