Markus Kraft

List of Publications by Year
in descending order

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351	13,516	22132	38368
papers	citations	59	95
		h-index	g-index

360	360	360	10839
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Blockchain technology in the chemical industry: Machine-to-machine electricity market. Applied Energy, 2017, 195, 234-246.	5.1	563
2	Nickel Nanoparticles Encapsulated in Fewâ€Layer Nitrogenâ€Doped Graphene Derived from Metalâ€“Organic Frameworks as Efficient Bifunctional Electrocatalysts for Overall Water Splitting. Advanced Materials, 2017, 29, 1605957.	11.1	507
3	Metal-free carbonaceous electrocatalysts and photocatalysts for water splitting. Chemical Society Reviews, 2016, 45, 3039-3052.	18.7	499
4	Unique Pï£¿Coï£¿N Surface Bonding States Constructed on gâ€C₃N₄ Nanosheets for Drastically Enhanced Photocatalytic Activity of H₂ Evolution. Advanced Functional Materials, 2017, 27, 1604328.	7.8	329
5	Investigating the Role of Tunable Nitrogen Vacancies in Graphitic Carbon Nitride Nanosheets for Efficient Visible-Light-Driven H₂ Evolution and CO₂ Reduction. ACS Sustainable Chemistry and Engineering, 2017, 5, 7260-7268.	3.2	322
6	Incorporating seller/buyer reputation-based system in blockchain-enabled emission trading application. Applied Energy, 2018, 209, 8-19.	5.1	271
7	Mapping surrogate gasoline compositions into RON/MON space. Combustion and Flame, 2010, 157, 1122-1131.	2.8	231
8	Measurement and numerical simulation of soot particle size distribution functions in a laminar premixed ethylene-oxygen-argon flame. Combustion and Flame, 2003, 133, 173-188.	2.8	230
9	Design of computer experiments: A review. Computers and Chemical Engineering, 2017, 106, 71-95.	2.0	215
10	A Highly Efficient Oxygen Evolution Catalyst Consisting of Interconnected Nickelâ€“Ironâ€Layered Double Hydroxide and Carbon Nanodomains. Advanced Materials, 2018, 30, 1705106.	11.1	209
11	A quantitative study of the clustering of polycyclic aromatic hydrocarbons at high temperatures. Physical Chemistry Chemical Physics, 2012, 14, 4081.	1.3	147
12	HRTEM evaluation of soot particles produced by the non-premixed combustion of liquid fuels. Carbon, 2016, 96, 459-473.	5.4	139
13	Towards a detailed soot model for internal combustion engines. Combustion and Flame, 2009, 156, 1156-1165.	2.8	137
14	Numerical simulation and sensitivity analysis of detailed soot particle size distribution in laminar premixed ethylene flames. Combustion and Flame, 2006, 145, 117-127.	2.8	130
15	Research advances towards large-scale solar hydrogen production from water. EnergyChem, 2019, 1, 100014.	10.1	130
16	Modelling the internal structure of nascent soot particles. Combustion and Flame, 2010, 157, 909-914.	2.8	126
17	Screening and techno-economic assessment of biomass-based power generation with CCS technologies to meet 2050 CO2 targets. Applied Energy, 2017, 190, 481-489.	5.1	126
18	A study on the coagulation of polycyclic aromatic hydrocarbon clusters to determine their collision efficiency. Combustion and Flame, 2010, 157, 523-534.	2.8	124

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19	Electronic and optical properties of aluminium-doped anatase and rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> initio</i>calculations. Physical Review B, 2010, 81, .	1.1	121
20	A statistical approach to develop a detailed soot growth model using PAH characteristics. Combustion and Flame, 2009, 156, 896-913.	2.8	117
21	Soot inception: Carbonaceous nanoparticle formation in flames. Progress in Energy and Combustion Science, 2022, 88, 100956.	15.8	117
22	A new model for the drying of droplets containing suspended solids. Chemical Engineering Science, 2009, 64, 628-637.	1.9	107
23	Investigation of combustion emissions in a homogeneous charge compression injection engine: Measurements and a new computational model. Proceedings of the Combustion Institute, 2000, 28, 1195-1201.	2.4	105
24	The impact of intelligent cyber-physical systems on the decarbonization of energy. Energy and Environmental Science, 2020, 13, 744-771.	15.6	104
25	Modelling soot formation in a premixed flame using an aromatic-site soot model and an improved oxidation rate. Proceedings of the Combustion Institute, 2009, 32, 639-646.	2.4	103
26	Internal structure of soot particles in a diffusion flame. Carbon, 2019, 141, 635-642.	5.4	94
27	Developing the PAH-PP soot particle model using process informatics and uncertainty propagation. Proceedings of the Combustion Institute, 2011, 33, 675-683.	2.4	91
28	The future viability of algae-derived biodiesel under economic and technical uncertainties. Bioresource Technology, 2014, 151, 166-173.	4.8	90
29	Quantitative tools for cultivating symbiosis in industrial parks; a literature review. Applied Energy, 2015, 155, 599-612.	5.1	89
30	An Efficient Stochastic Algorithm for Simulating Nano-particle Dynamics. Journal of Computational Physics, 2002, 183, 210-232.	1.9	85
31	Numerical simulations of soot aggregation in premixed laminar flames. Proceedings of the Combustion Institute, 2007, 31, 693-700.	2.4	83
32	The carbon footprint and non-renewable energy demand of algae-derived biodiesel. Applied Energy, 2014, 113, 1632-1644.	5.1	83
33	Applying Industry 4.0 to the Jurong Island Eco-industrial Park. Energy Procedia, 2015, 75, 1536-1541.	1.8	83
34	Stochastic modeling of soot particle size and age distributions in laminar premixed flames. Proceedings of the Combustion Institute, 2005, 30, 1457-1465.	2.4	82
35	Modelling soot formation from wall films in a gasoline direct injection engine using a detailed population balance model. Applied Energy, 2016, 163, 154-166.	5.1	82
36	A fully coupled simulation of PAH and soot growth with a population balance model. Proceedings of the Combustion Institute, 2013, 34, 1827-1835.	2.4	81

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37	Coupling a stochastic soot population balance to gas-phase chemistry using operator splitting. Combustion and Flame, 2007, 148, 158-176.	2.8	78
38	Models for the aggregate structure of soot particles. Combustion and Flame, 2007, 151, 160-172.	2.8	77
39	Detailed modeling of soot formation in a partially stirred plug flow reactor. Combustion and Flame, 2002, 128, 395-409.	2.8	75
40	Aromatic site description of soot particles. Combustion and Flame, 2008, 155, 161-180.	2.8	73
41	Simulating the structural evolution of droplets following shell formation. Chemical Engineering Science, 2010, 65, 713-725.	1.9	72
42	Toward a Comprehensive Model of the Synthesis of TiO₂ Particles from TiCl₄. Industrial & Engineering Chemistry Research, 2007, 46, 6147-6156.	1.8	70
43	PAH structure analysis of soot in a non-premixed flame using high-resolution transmission electron microscopy and optical band gap analysis. Combustion and Flame, 2016, 164, 250-258.	2.8	69
44	The evolution of the biofuel science. Renewable and Sustainable Energy Reviews, 2017, 76, 1479-1484.	8.2	69
45	First-Principles Thermochemistry for the Production of TiO2from TiCl4. Journal of Physical Chemistry A, 2007, 111, 3560-3565.	1.1	66
46	A Detailed Model for the Sintering of Polydispersed Nanoparticle Agglomerates. Aerosol Science and Technology, 2009, 43, 978-989.	1.5	66
47	Design technologies for eco-industrial parks: From unit operations to processes, plants and industrial networks. Applied Energy, 2016, 175, 305-323.	5.1	66
48	The Linear Process Deferment Algorithm: A new technique for solving population balance equations. SIAM Journal of Scientific Computing, 2006, 28, 303-320.	1.3	65
49	Size-dependent melting of polycyclic aromatic hydrocarbon nano-clusters: A molecular dynamics study. Carbon, 2014, 67, 79-91.	5.4	65
50	A new numerical approach for the simulation of the growth of inorganic nanoparticles. Journal of Computational Physics, 2006, 211, 638-658.	1.9	64
51	A new model for the drying of droplets containing suspended solids after shell formation. Chemical Engineering Science, 2009, 64, 228-246.	1.9	64
52	New polycyclic aromatic hydrocarbon (PAH) surface processes to improve the model prediction of the composition of combustion-generated PAHs and soot. Carbon, 2010, 48, 319-332.	5.4	64
53	A coupled CFD-population balance approach for nanoparticle synthesis in turbulent reacting flows. Chemical Engineering Science, 2011, 66, 3792-3805.	1.9	64
54	Smart Sampling Algorithm for Surrogate Model Development. Computers and Chemical Engineering, 2017, 96, 103-114.	2.0	63

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55	Wetting-regulated gas-involving (photo)electrocatalysis: biomimetics in energy conversion. Chemical Society Reviews, 2021, 50, 10674-10699.	18.7	63
56	Extending stochastic soot simulation to higher pressures. Combustion and Flame, 2006, 145, 638-642.	2.8	62
57	A First Principles Development of a General Anisotropic Potential for Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2010, 6, 683-695.	2.3	62
58	Sooting characteristics of polyoxymethylene dimethyl ether blends with diesel in a diffusion flame. Fuel, 2018, 224, 499-506.	3.4	62
59	The simultaneous reduction of nitric oxide and soot in emissions from diesel engines. Carbon, 2009, 47, 866-875.	5.4	61
60	Modelling the flame synthesis of silica nanoparticles from tetraethoxysilane. Chemical Engineering Science, 2012, 70, 54-66.	1.9	61
61	Sooting tendency of paraffin components of diesel and gasoline in diffusion flames. Fuel, 2014, 126, 8-15.	3.4	60
62	Parameter estimation in a multidimensional granulation model. Powder Technology, 2010, 197, 196-210.	2.1	59
63	Modelling and validation of granulation with heterogeneous binder dispersion and chemical reaction. Chemical Engineering Science, 2007, 62, 4717-4728.	1.9	57
64	Numerical simulation and parametric sensitivity study of particle size distributions in a burner-stabilised stagnation flame. Combustion and Flame, 2015, 162, 2569-2581.	2.8	57
65	Stochastic weighted particle methods for population balance equations. Journal of Computational Physics, 2011, 230, 7456-7472.	1.9	56
66	Dual injection homogeneous charge compression ignition engine simulation using a stochastic reactor model. International Journal of Engine Research, 2007, 8, 41-50.	1.4	55
67	Sooting tendency and particle size distributions of n-heptane/toluene mixtures burned in a wick-fed diffusion flame. Fuel, 2016, 169, 111-119.	3.4	55
68	A mechanistic study on the simultaneous elimination of soot and nitric oxide from engine exhaust. Carbon, 2011, 49, 1516-1531.	5.4	52
69	An improved methodology for determining threshold sooting indices from smoke point lamps. Fuel, 2013, 111, 120-130.	3.4	52
70	Sooting tendency of surrogates for the aromatic fractions of diesel and gasoline in a wick-fed diffusion flame. Fuel, 2015, 153, 31-39.	3.4	52
71	Modelling of a RDC using a combined CFD-population balance approach. Chemical Engineering Science, 2004, 59, 2597-2606.	1.9	51
72	Influence of Injection Timing and Piston Bowl Geometry on PCCI Combustion and Emissions. SAE International Journal of Engines, 0, 2, 1019-1033.	0.4	50

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73	A detailed kinetic model for combustion synthesis of titania from TiCl4. Combustion and Flame, 2009, 156, 1764-1770.	2.8	49
74	Techno-economic assessment of carbon-negative algal biodiesel for transport solutions. Applied Energy, 2013, 106, 262-274.	5.1	49
75	Knowledge management of eco-industrial park for efficient energy utilization through ontology-based approach. Applied Energy, 2017, 204, 1412-1421.	5.1	49
76	Iterative improvement of Bayesian parameter estimates for an engine model by means of experimental design. Combustion and Flame, 2012, 159, 1303-1313.	2.8	48
77	The Polarization of Polycyclic Aromatic Hydrocarbons Curved by Pentagon Incorporation: The Role of the Flexoelectric Dipole. Journal of Physical Chemistry C, 2017, 121, 27154-27163.	1.5	48
78	Manipulating Intermediates at the Auâ€“TiO₂ Interface over InP Nanopillar Array for Photoelectrochemical CO₂ Reduction. ACS Catalysis, 2021, 11, 11416-11428.	5.5	48
79	Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Implications of Localized Ï€-Radicals on Rim-Based Pentagonal Rings. Journal of Physical Chemistry C, 2019, 123, 26673-26682.	1.5	47
80	OntoKin: An Ontology for Chemical Kinetic Reaction Mechanisms. Journal of Chemical Information and Modeling, 2020, 60, 108-120.	2.5	47
81	Sources of CO emissions in an HCCI engine: A numerical analysis. Combustion and Flame, 2006, 144, 634-637.	2.8	46
82	Optical band gap of cross-linked, curved, and radical polyaromatic hydrocarbons. Physical Chemistry Chemical Physics, 2019, 21, 16240-16251.	1.3	45
83	A multidimensional population balance model to describe the aerosol synthesis of silica nanoparticles. Journal of Aerosol Science, 2012, 44, 83-98.	1.8	44
84	Homogeneous Charge Compression Ignition Engine: A Simulation Study on the Effects of Inhomogeneities. Journal of Engineering for Gas Turbines and Power, 2003, 125, 466-471.	0.5	43
85	Numerical investigation of DQMoM-IEM as a turbulent reaction closure. Chemical Engineering Science, 2010, 65, 1915-1924.	1.9	43
86	A novel methodology for the design of waste heat recovery network in eco-industrial park using techno-economic analysis and multi-objective optimization. Applied Energy, 2016, 184, 88-102.	5.1	43
87	An agent composition framework for the J-Park Simulator - A knowledge graph for the process industry. Computers and Chemical Engineering, 2019, 130, 106577.	2.0	43
88	J-Park Simulator: An ontology-based platform for cross-domain scenarios in process industry. Computers and Chemical Engineering, 2019, 131, 106586.	2.0	43
89	Investigation of the impact of the configuration of exhaust after-treatment system for diesel engines. Applied Energy, 2020, 267, 114844.	5.1	43
90	Universal Digital Twin - A Dynamic Knowledge Graph. Data-Centric Engineering, 2021, 2, .	1.2	43

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91	A computational study of an HCCI engine with direct injection during gas exchange. Combustion and Flame, 2006, 147, 118-132.	2.8	42
92	Stochastic weighted particle methods for population balance equations with coagulation, fragmentation and spatial inhomogeneity. Journal of Computational Physics, 2015, 303, 1-18.	1.9	42
93	An ontology framework towards decentralized information management for eco-industrial parks. Computers and Chemical Engineering, 2018, 118, 49-63.	2.0	42
94	Modelling particle mass and particle number emissions during the active regeneration of diesel particulate filters. Proceedings of the Combustion Institute, 2019, 37, 4831-4838.	2.4	42
95	From Platform to Knowledge Graph: Evolution of Laboratory Automation. Jacs Au, 2022, 2, 292-309.	3.6	42
96	Real-Time Evaluation of a Detailed Chemistry HCCI Engine Model Using a Tabulation Technique. Combustion Science and Technology, 2008, 180, 1263-1277.	1.2	41
97	Ï€-Diradical Aromatic Soot Precursors in Flames. Journal of the American Chemical Society, 2021, 143, 12212-12219.	6.6	41
98	Evaluating the EGR-AFR Operating Range of a HCCI Engine. , 2005, , .		40
99	Polymorphism of nanocrystalline TiO₂ prepared in a stagnation flame: formation of the TiO₂-II phase. Chemical Science, 2019, 10, 1342-1350.	3.7	40
100	Experimental and numerical study of the evolution of soot primary particles in a diffusion flame. Proceedings of the Combustion Institute, 2019, 37, 2047-2055.	2.4	39
101	Bayesian Error Propagation for a Kinetic Model of nâ€Propylbenzene Oxidation in a Shock Tube. International Journal of Chemical Kinetics, 2014, 46, 389-404.	1.0	38
102	First-Principles Thermochemistry for Silicon Species in the Decomposition of Tetraethoxysilane. Journal of Physical Chemistry A, 2009, 113, 9041-9049.	1.1	37
103	Modelling soot formation in a DISI engine. Proceedings of the Combustion Institute, 2011, 33, 3159-3167.	2.4	37
104	Giant fullerene formation through thermal treatment of fullerene soot. Carbon, 2017, 125, 132-138.	5.4	37
105	Polar curved polycyclic aromatic hydrocarbons in soot formation. Proceedings of the Combustion Institute, 2019, 37, 1117-1123.	2.4	37
106	Topology of Disordered 3D Graphene Networks. Physical Review Letters, 2019, 123, 116105.	2.9	37
107	Game theory-based renewable multi-energy system design and subsidy strategy optimization. Advances in Applied Energy, 2021, 2, 100024.	6.6	37
108	Simulation of coalescence and breakage: an assessment of two stochastic methods suitable for simulating liquidâ€“liquid extraction. Chemical Engineering Science, 2004, 59, 3865-3881.	1.9	36

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109	Modelling soot formation in a benchmark ethylene stagnation flame with a new detailed population balance model. Combustion and Flame, 2019, 203, 56-71.	2.8	36
110	Solidâ€“liquid transitions in homogenous ovalene, hexabenzocoronene and circumcoronene clusters: A molecular dynamics study. Combustion and Flame, 2015, 162, 486-495.	2.8	35
111	Soot particle size distributions in premixed stretch-stabilized flat ethyleneâ€“oxygenâ€“argon flames. Proceedings of the Combustion Institute, 2017, 36, 1001-1009.	2.4	35
112	Partially Stirred Reactor Model: Analytical Solutions and Numerical Convergence Study of a PDF/Monte Carlo Method. SIAM Journal of Scientific Computing, 2004, 25, 1798-1823.	1.3	33
113	NOx and N2O formation in HCCI engines. , 2005, , .		33
114	A kinetic mechanism for the thermal decomposition of titanium tetraisopropoxide. Proceedings of the Combustion Institute, 2017, 36, 1019-1027.	2.4	33
115	Extension of moment projection method to the fragmentation process. Journal of Computational Physics, 2017, 335, 516-534.	1.9	33
116	An Ontology and Semantic Web Service for Quantum Chemistry Calculations. Journal of Chemical Information and Modeling, 2019, 59, 3154-3165.	2.5	33
117	Simulating a Homogeneous Charge Compression Ignition Engine Fuelled with a DEE/EtOH Blend. , 0, , .		32
118	Droplets population balance in a rotating disc contactor: An inverse problem approach. AICHE Journal, 2006, 52, 1441-1450.	1.8	32
119	On a multivariate population balance model to describe the structure and composition of silica nanoparticles. Computers and Chemical Engineering, 2012, 43, 130-147.	2.0	32
120	Stochastic solution of population balance equations for reactor networks. Journal of Computational Physics, 2014, 256, 615-629.	1.9	32
121	Rational Synthesis of Amorphous Ironâ€Nickel Phosphonates for Highly Efficient Photocatalytic Water Oxidation with Almost 100â€‰% Yield. Angewandte Chemie - International Edition, 2020, 59, 1171-1175.	7.2	32
122	Improved methodology for performing the inverse Abel transform of flame images for color ratio pyrometry. Applied Optics, 2019, 58, 2662.	0.9	32
123	First-Principles Thermochemistry for the Thermal Decomposition of Titanium Tetraisopropoxide. Journal of Physical Chemistry A, 2015, 119, 8376-8387.	1.1	31
124	Towards an ontological infrastructure for chemical process simulation and optimization in the context of eco-industrial parks. Applied Energy, 2017, 204, 1284-1298.	5.1	31
125	OntoPowSys: A power system ontology for cross domain interactions in an eco industrial park. Energy and AI, 2020, 1, 100008.	5.8	31
126	On the thermophoretic sampling and TEM-based characterisation of soot particles in flames. Carbon, 2021, 171, 711-722.	5.4	31

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127	Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation. Journal of Computational Physics, 2010, 229, 7672-7691.	1.9	30
128	Phase change of polycyclic aromatic hydrocarbon clusters by mass addition. Carbon, 2014, 77, 25-35.	5.4	30
129	Modelling a Dual-Fuelled Multi-Cylinder HCCI Engine Using a PDF Based Engine Cycle Simulator. , 0, , .		29
130	A Monte Carlo methods for identification and sensitivity analysis of coagulation processes. Journal of Computational Physics, 2004, 200, 50-59.	1.9	29
131	Incorporating experimental uncertainties into multivariate granulation modelling. Chemical Engineering Science, 2010, 65, 1088-1100.	1.9	29
132	Statistical Approximation of the Inverse Problem in Multivariate Population Balance Modeling. Industrial & Engineering Chemistry Research, 2010, 49, 428-438.	1.8	29
133	Delivering authentic experiences for engineering students and professionals through e-labs. , 2010, , .		29
134	Simulation and life cycle assessment of algae gasification process in dual fluidized bed gasifiers. Green Chemistry, 2015, 17, 1793-1801.	4.6	29
135	From database to knowledge graph â€" using data in chemistry. Current Opinion in Chemical Engineering, 2019, 26, 33-37.	3.8	29
136	On the coagulation efficiency of carbonaceous nanoparticles. Journal of Aerosol Science, 2020, 140, 105478.	1.8	29
137	Adsorption, Diffusion and Desorption of Chlorine on and from Rutile TiO2{110}: A Theoretical Investigation. ChemPhysChem, 2007, 8, 444-451.	1.0	28
138	A transferable electrostatic model for intermolecular interactions between polycyclic aromatic hydrocarbons. Chemical Physics Letters, 2011, 510, 154-160.	1.2	28
139	A new model for silicon nanoparticle synthesis. Combustion and Flame, 2013, 160, 947-958.	2.8	28
140	Modelling PAH curvature in laminar premixed flames using a detailed population balance model. Combustion and Flame, 2017, 176, 172-180.	2.8	28
141	LEAPS2: Learning based Evolutionary Assistive Paradigm for Surrogate Selection. Computers and Chemical Engineering, 2018, 119, 352-370.	2.0	28
142	Optimal site selection for modular nuclear power plants. Computers and Chemical Engineering, 2019, 125, 339-350.	2.0	28
143	Flame Synthesized Blue TiO_{2â^'}_x with Tunable Oxygen Vacancies from Surface to Grain Boundary to Bulk. Small Methods, 2021, 5, e2000928.	4.6	28
144	The future of computational modelling in reaction engineering. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3633-3644.	1.6	27

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145	A virtual laboratory to support chemical reaction engineering courses using real-life problems and industrial software. Education for Chemical Engineers, 2020, 33, 36-44.	2.8	27
146	Modelling nanoparticle dynamics: coagulation, sintering, particle inception and surface growth. Combustion Theory and Modelling, 2005, 9, 449-461.	1.0	26
147	The inverse problem in granulation modelingâ€"Two different statistical approaches. AICHE Journal, 2011, 57, 3105-3121.	1.8	26
148	Production of Biorenewable Hydrogen and Syngas via Algae Gasification: A Sensitivity Analysis. Energy Procedia, 2014, 61, 2767-2770.	1.8	26
149	Modelling TiO 2 formation in a stagnation flame using method of moments with interpolative closure. Combustion and Flame, 2017, 178, 135-147.	2.8	26
150	Knowledge Graph Approach to Combustion Chemistry and Interoperability. ACS Omega, 2020, 5, 18342-18348.	1.6	26
151	Semantic 3D City Database â€" An enabler for a dynamic geospatial knowledge graph. Energy and AI, 2021, 6, 100106.	5.8	26
152	Bayesian parameter estimation for a jet-milling model using Metropolisâ€"Hastings and Wangâ€"Landau sampling. Chemical Engineering Science, 2013, 89, 244-257.	1.9	25
153	Numerical simulation and parametric sensitivity study of optical band gap in a laminar co-flow ethylene diffusion flame. Combustion and Flame, 2016, 167, 320-334.	2.8	25
154	Self-template synthesis of CdS/NiS_x heterostructured nanohybrids for efficient photocatalytic hydrogen evolution. Dalton Transactions, 2017, 46, 10650-10656.	1.6	25
155	Premixed Stagnation Flame Synthesized TiO₂ Nanoparticles with Mixed Phases for Efficient Photocatalytic Hydrogen Generation. ACS Sustainable Chemistry and Engineering, 2018, 6, 14470-14479.	3.2	25
156	Box-Behnken design based CO2 co-gasification of horticultural waste and sewage sludge with addition of ash from waste as catalyst. Applied Energy, 2019, 242, 1549-1561.	5.1	25
157	Reactivity of Polycyclic Aromatic Hydrocarbon Soot Precursors: Kinetics and Equilibria. Journal of Physical Chemistry A, 2020, 124, 10040-10052.	1.1	25
158	The impact of cyclic fuels on the formation and structure of soot. Combustion and Flame, 2020, 219, 1-12.	2.8	25
159	Assessing the Polycyclic Aromatic Hydrocarbon Anisotropic Potential with Application to the Exfoliation Energy of Graphite. Journal of Physical Chemistry A, 2011, 115, 13684-13693.	1.1	24
160	The semantics of Chemical Markup Language (CML) for computational chemistry : CompChem. Journal of Cheminformatics, 2012, 4, 15.	2.8	24
161	Parameterisation of a biodiesel plant process flow sheet model. Computers and Chemical Engineering, 2016, 95, 108-122.	2.0	24
162	Development of a multi-compartment population balance model for high-shear wet granulation with discrete element method. Computers and Chemical Engineering, 2017, 99, 171-184.	2.0	24

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163	A moment projection method for population balance dynamics with a shrinkage term. Journal of Computational Physics, 2017, 330, 960-980.	1.9	24
164	Emerging applications of nanocatalysts synthesized by flame aerosol processes. Current Opinion in Chemical Engineering, 2018, 20, 39-49.	3.8	24
165	First-Principles Thermochemistry for the Combustion of a TiCl4 and AlCl3 Mixture. Journal of Physical Chemistry A, 2009, 113, 13790-13796.	1.1	23
166	Comparison of the stochastic fields method and DQMoM-IEM as turbulent reaction closures. Chemical Engineering Science, 2010, 65, 5429-5441.	1.9	23
167	Experimental Investigation of a Control Method for SI-HCCI-SI Transition in a Multi-Cylinder Gasoline Engine. SAE International Journal of Engines, 0, 3, 928-937.	0.4	23
168	Implementing Detailed Chemistry and In-Cylinder Stratification into 0/1-D IC Engine Cycle Simulation Tools. , 0, , .		23
169	Modelling cycle to cycle variations in an SI engine with detailed chemical kinetics. Combustion and Flame, 2011, 158, 179-188.	2.8	23
170	Surface reactivity of polycyclic aromatic hydrocarbon clusters. Proceedings of the Combustion Institute, 2015, 35, 1811-1818.	2.4	23
171	A detailed kinetic study of the thermal decomposition of tetraethoxysilane. Proceedings of the Combustion Institute, 2015, 35, 2291-2298.	2.4	23
172	Detailed population balance modelling of TiO 2 synthesis in an industrial reactor. Chemical Engineering Science, 2017, 164, 219-231.	1.9	23
173	Flexoelectricity and the Formation of Carbon Nanoparticles in Flames. Journal of Physical Chemistry C, 2018, 122, 22210-22215.	1.5	23
174	The effect of poly(oxymethylene) dimethyl ethers (PODE3) on soot formation in ethylene/PODE3 laminar coflow diffusion flames. Fuel, 2021, 283, 118769.	3.4	23
175	A Detailed Chemistry Multi-cycle Simulation of a Gasoline Fueled HCCI Engine Operated with NVO. SAE International Journal of Fuels and Lubricants, 0, 2, 13-27.	0.2	22
176	Theoretical insights into the surface growth of rutile TiO2. Combustion and Flame, 2011, 158, 1868-1876.	2.8	22
177	Microkinetic Modeling of the Fischerâ€“Tropsch Synthesis over Cobalt Catalysts. ChemCatChem, 2015, 7, 137-143.	1.8	22
178	Exploring the internal structure of soot particles using nanoindentation: A reactive molecular dynamics study. Combustion and Flame, 2020, 219, 45-56.	2.8	22
179	Two-stage Fuel Direct Injection in a Diesel Fuelled HCCI Engine. , 0, , .		21
180	From Numerical Model to Computational Intelligence: The Digital Transition of Urban Energy System. Energy Procedia, 2017, 143, 884-890.	1.8	21

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181	An adsorption-precipitation model for the formation of injector external deposits in internal combustion engines. Applied Energy, 2018, 228, 1423-1438.	5.1	21
182	Ion-Induced Soot Nucleation Using a New Potential for Curved Aromatics. Combustion Science and Technology, 2019, 191, 747-765.	1.2	21
183	Studying the Influence of Direct Injection on PCCI Combustion and Emissions at Engine Idle Condition Using Two Dimensional CFD and Stochastic Reactor Model. , 2008, , .		20
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