Guy B Marin

List of Publications by Year
in descending order

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502 papers	21,801 citations	10979 71 h-index	22808 112 g-index
514 all docs	514 docs citations	514 times ranked	15970 citing authors

#	Article	IF	Citations
1	Determination of the V2p XPS binding energies for different vanadium oxidation states (V5+ to V0+). Journal of Electron Spectroscopy and Related Phenomena, 2004, 135, 167-175.	0.8	1,420
2	New Trends in Olefin Production. Engineering, 2017, 3, 171-178.	3.2	512
3	Enhanced Carbon-Resistant Dry Reforming Fe-Ni Catalyst: RoleÂofÂFe. ACS Catalysis, 2015, 5, 3028-3039.	5.5	383
4	Super-dry reforming of methane intensifies CO ₂ utilization via Le Chatelierâ€™s principle. Science, 2016, 354, 449-452.	6.0	348
5	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. Combustion and Flame, 2011, 158, 16-41.	2.8	240
6	Modeling the evaporation of a hydrocarbon feedstock in the convection section of a steam cracker. Computers and Chemical Engineering, 2009, 33, 122-132.	2.0	224
7	Simulation of heterogeneously MgO-catalyzed transesterification for fine-chemical and biodiesel industrial production. Applied Catalysis B: Environmental, 2006, 67, 136-148.	10.8	217
8	Kinetics of heterogeneously MgO-catalyzed transesterification. Applied Catalysis B: Environmental, 2006, 62, 35-45.	10.8	190
9	Adsorption of C2â^'C8 n-Alkanes in Zeolites. Journal of Physical Chemistry C, 2011, 115, 1204-1219.	1.5	187
10	The strength of multi-scale modeling to unveil the complexity of radical polymerization. Progress in Polymer Science, 2016, 58, 59-89.	11.8	174
11	The Chemical Route to a Carbon Dioxide Neutral World. ChemSusChem, 2017, 10, 1039-1055.	3.6	174
12	Carbon gasification from Feâ€“Ni catalysts after methane dry reforming. Applied Catalysis B: Environmental, 2016, 185, 42-55.	10.8	173
13	Ab Initio Calculations for Hydrocarbons:Â Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. Journal of Physical Chemistry A, 2003, 107, 9147-9159.	1.1	170
14	Density Functional Study of Benzene Adsorption on Pt(111). Journal of Physical Chemistry B, 2002, 106, 7489-7498.	1.2	166
15	Zeolite Shape-Selectivity in thegem-Methylation of Aromatic Hydrocarbons. Angewandte Chemie - International Edition, 2007, 46, 1311-1314.	7.2	154
16	First Principle Kinetic Studies of Zeolite-Catalyzed Methylation Reactions. Journal of the American Chemical Society, 2011, 133, 888-899.	6.6	153
17	CeO₂-Modified Fe₂O₃ for CO₂ Utilization via Chemical Looping. Industrial & Engineering Chemistry Research, 2013, 52, 8416-8426.	1.8	149
18	Microkinetics of methane oxidative coupling. Catalysis Today, 2008, 137, 90-102.	2.2	145

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19	Linear Gradient Quality of ATRP Copolymers. Macromolecules, 2012, 45, 8519-8531.	2.2	139
20	Theoretical Study of the Thermodynamics and Kinetics of Hydrogen Abstractions from Hydrocarbons. Journal of Physical Chemistry A, 2007, 111, 11771-11786.	1.1	134
21	Theoretical Insights on Methylbenzene Sideâ€Chain Growth in ZSMâ€5 Zeolites for Methanolâ€toâ€Olefin Conversion. Chemistry - A European Journal, 2009, 15, 10803-10808.	1.7	131
22	Eurokin. Chemical Reaction Kinetics in Practice. Cattech, 2001, 5, 36-60.	2.6	127
23	Group Additive Values for the Gas Phase Standard Enthalpy of Formation of Hydrocarbons and Hydrocarbon Radicals. Journal of Physical Chemistry A, 2005, 109, 7466-7480.	1.1	127
24	Acidâ^'Metal Balance of a Hydrocracking Catalyst:Â Ideal versus Nonideal Behavior. Industrial & Engineering Chemistry Research, 2005, 44, 5159-5169.	1.8	125
25	An XPS study on the surface reduction of V2O5(001) induced by Ar+ ion bombardment. Surface Science, 2006, 600, 3512-3517.	0.8	124
26	The Crucial Role of Diffusional Limitations in Controlled Radical Polymerization. Macromolecular Reaction Engineering, 2013, 7, 362-379.	0.9	122
27	Automatic reaction network generation using RMG for steam cracking of n-hexane. AICHE Journal, 2006, 52, 718-730.	1.8	119
28	Genesys: Kinetic model construction using chemo-informatics. Chemical Engineering Journal, 2012, 207-208, 526-538.	6.6	116
29	Catalyst-assisted chemical looping for CO2 conversion to CO. Applied Catalysis B: Environmental, 2015, 164, 184-191.	10.8	110
30	Characterization and Comparison of Fast Pyrolysis Bio-oils from Pinewood, Rapeseed Cake, and Wheat Straw Using ¹³C NMR and Comprehensive GC Ã— GC. ACS Sustainable Chemistry and Engineering, 2016, 4, 4974-4985.	3.2	109
31	Physisorption and chemisorption of alkanes and alkenes in H-FAU: a combined ab initioâ€“statistical thermodynamics study. Physical Chemistry Chemical Physics, 2009, 11, 2939.	1.3	104
32	Development of a transient kinetic model for the CO oxidation by O2 over a Pt/Rh/CeO2/Î³-Al2O3 three-way catalyst. Applied Catalysis B: Environmental, 1998, 19, 245-259.	10.8	103
33	Making chemicals with electricity. Science, 2019, 364, 734-735.	6.0	102
34	The coordinatively saturated vanadium MIL-47 as a low leaching heterogeneous catalyst in the oxidation of cyclohexene. Journal of Catalysis, 2012, 285, 196-207.	3.1	100
35	Delivering a Modifying Element to Metal Nanoparticles via Support: Ptâ€“Ga Alloying during the Reduction of Pt/Mg(Al,Ga)O_x Catalysts and Its Effects on Propane Dehydrogenation. ACS Catalysis, 2014, 4, 1812-1824.	5.5	100
36	Dynamic methods for catalytic kinetics. Applied Catalysis A: General, 2008, 342, 3-28.	2.2	99

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37	Comprehensive compositional analysis of sulfur and nitrogen containing compounds in shale oil using GCÃ—GC â€“ FID/SCD/NCD/TOF-MS. Fuel, 2015, 140, 398-406.	3.4	99
38	The Rise and Fall of Direct Mechanisms in Methanol-to-Olefin Catalysis:Â An Overview of Theoretical Contributions. Industrial & Engineering Chemistry Research, 2007, 46, 8832-8838.	1.8	95
39	The Positive Role of Hydrogen on the Dehydrogenation of Propane on Pt(111). ACS Catalysis, 2017, 7, 7495-7508.	5.5	95
40	Normal Mode Analysis in Zeolites: Toward an Efficient Calculation of Adsorption Entropies. Journal of Chemical Theory and Computation, 2011, 7, 1090-1101.	2.3	94
41	Automatic Mechanism and Kinetic Model Generation for Gasâ€•and Solutionâ€Phase Processes: A Perspective on Best Practices, Recent Advances, and Future Challenges. International Journal of Chemical Kinetics, 2015, 47, 199-231.	1.0	94
42	Model-based design of the polymer microstructure: bridging the gap between polymer chemistry and engineering. Polymer Chemistry, 2015, 6, 7081-7096.	1.9	94
43	On-line analysis of complex hydrocarbon mixtures using comprehensive two-dimensional gas chromatography. Journal of Chromatography A, 2010, 1217, 6623-6633.	1.8	90
44	ARGET ATRP of Butyl Methacrylate: Utilizing Kinetic Modeling To Understand Experimental Trends. Macromolecules, 2013, 46, 3828-3840.	2.2	90
45	Low-Temperature Atomic Layer Deposition of Platinum Using (Methylcyclopentadienyl)trimethylplatinum and Ozone. Journal of Physical Chemistry C, 2013, 117, 20557-20561.	1.5	90
46	Controlling the stability of a Feâ€“Ni reforming catalyst: Structural organization of the active components. Applied Catalysis B: Environmental, 2017, 209, 405-416.	10.8	89
47	Ab initio group contribution method for activation energies for radical additions. AICHE Journal, 2004, 50, 426-444.	1.8	88
48	Ethanol to higher hydrocarbons over Ni, Ga, Fe-modified ZSM-5: Effect of metal content. Applied Catalysis A: General, 2015, 492, 117-126.	2.2	88
49	Upgrading the value of anaerobic digestion via chemical production from grid injected biomethane. Energy and Environmental Science, 2018, 11, 1788-1802.	15.6	88
50	Carbonâ€Centered Radical Addition and Î²â€Scission Reactions: Modeling of Activation Energies and Preâ€exponential Factors. ChemPhysChem, 2008, 9, 124-140.	1.0	87
51	First Principles Based Group Additive Values for the Gas Phase Standard Entropy and Heat Capacity of Hydrocarbons and Hydrocarbon Radicals. Journal of Physical Chemistry A, 2008, 112, 12235-12251.	1.1	86
52	Methodology for Kinetic Modeling of Atom Transfer Radical Polymerization. Macromolecular Reaction Engineering, 2009, 3, 185-209.	0.9	85
53	Modeling fast biomass pyrolysis in a gasâ€“solid vortex reactor. Chemical Engineering Journal, 2012, 207-208, 195-208.	6.6	85
54	Advanced Chemical Looping Materials for CO2 Utilization: A Review. Materials, 2018, 11, 1187.	1.3	85

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55	Molecular reconstruction of naphtha steam cracking feedstocks based on commercial indices. Computers and Chemical Engineering, 2007, 31, 1020-1034.	2.0	84
56	Origin of the Difference between Branching in Acrylates Polymerization under Controlled and Free Radical Conditions: A Computational Study of Competitive Processes. Macromolecules, 2011, 44, 8361-8373.	2.2	84
57	Reaction network for the total oxidation of toluene over CuOâ€“CeO2/Al2O3. Journal of Catalysis, 2011, 283, 1-9.	3.1	84
58	Catalyst design based on microkinetic models: Oxidative coupling of methane. Catalysis Today, 2011, 159, 29-36.	2.2	84
59	Kinetic Modeling of ICAR ATRP. Macromolecular Theory and Simulations, 2012, 21, 52-69.	0.6	84
60	The thermal decomposition of 2,5-dimethylfuran. Proceedings of the Combustion Institute, 2013, 34, 251-258.	2.4	80
61	Influence of Dimethyl Disulfide on Coke Formation during Steam Cracking of Hydrocarbons. Industrial & Engineering Chemistry Research, 2007, 46, 4134-4148.	1.8	78
62	Nature of the active sites for the total oxidation of toluene by CuOCeO2/Al2O3. Journal of Catalysis, 2012, 295, 91-103.	3.1	78
63	Kinetic Modeling of Radical Thiolâ€“Ene Chemistry for Macromolecular Design: Importance of Side Reactions and Diffusional Limitations. Macromolecules, 2013, 46, 1732-1742.	2.2	78
64	Experimental and modeling study of the pyrolysis and combustion of dimethoxymethane. Combustion and Flame, 2018, 190, 270-283.	2.8	78
65	Formation of ZSMâ€22 Zeolite Catalytic Particles by Fusion of Elementary Nanorods. Chemistry - A European Journal, 2007, 13, 10070-10077.	1.7	77
66	Anharmonicity and Confinement in Zeolites: Structure, Spectroscopy, and Adsorption Free Energy of Ethanol in H-ZSM-5. Journal of Physical Chemistry C, 2016, 120, 7172-7182.	1.5	77
67	The role of CO2 in the dehydrogenation of propane over WO â€“VO /SiO2. Journal of Catalysis, 2016, 335, 1-10.	3.1	77
68	Tracer Chromatographic Study of Pore and Pore Mouth Adsorption of Linear and Monobranched Alkanes on ZSM-22 Zeolite. Journal of Physical Chemistry B, 2003, 107, 398-406.	1.2	76
69	An experimental and kinetic modeling study of cyclopentadiene pyrolysis: First growth of polycyclic aromatic hydrocarbons. Combustion and Flame, 2014, 161, 2739-2751.	2.8	75
70	Biomass to olefins: Cracking of renewable naphtha. Chemical Engineering Journal, 2011, 176-177, 178-187.	6.6	74
71	Single-Event Microkinetics for Methanol to Olefins on H-ZSM-5. Industrial & Engineering Chemistry Research, 2013, 52, 1491-1507.	1.8	73
72	Density Functional Theory Analysis of Benzene (De)hydrogenation on Pt(111):Â Addition and Removal of the First Two H-Atoms. Journal of Physical Chemistry B, 2003, 107, 3844-3855.	1.2	71

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73	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. Industrial & Engineering Chemistry Research, 2010, 49, 10399-10420.	1.8	71
74	Reaction path analysis of propane selective oxidation over V2O5 and V2O5/TiO2. Journal of Catalysis, 2012, 289, 127-139.	3.1	71
75	Detailed compositional characterization of plastic waste pyrolysis oil by comprehensive two-dimensional gas-chromatography coupled to multiple detectors. Journal of Chromatography A, 2014, 1359, 237-246.	1.8	70
76	Mgâ€“Feâ€“Alâ€“O for advanced CO₂to CO conversion: carbon monoxide yield vs. oxygen storage capacity. Journal of Materials Chemistry A, 2015, 3, 16251-16262.	5.2	70
77	First principleâ€based simulation of ethane steam cracking. AICHE Journal, 2011, 57, 482-496.	1.8	69
78	DFT-based microkinetic modeling of ethanol dehydration in H-ZSM-5. Journal of Catalysis, 2016, 339, 173-185.	3.1	69
79	Theoretical study of the adsorption of C1â€“C4 primary alcohols in H-ZSM-5. Physical Chemistry Chemical Physics, 2010, 12, 9481.	1.3	68
80	The effect of bismuth on the selective oxidation of lactose on supported palladium catalysts. Carbohydrate Research, 1990, 204, 121-129.	1.1	67
81	Ab Initio Thermochemistry and Kinetics for Carbon-Centered Radical Addition and Î²-Scission Reactions. Journal of Physical Chemistry A, 2007, 111, 8416-8428.	1.1	67
82	Kinetic modeling of the total oxidation of propane over CuO-CeO2/Î³-Al2O3. Applied Catalysis B: Environmental, 2010, 95, 26-38.	10.8	67
83	Improved Livingness and Control over Branching in RAFT Polymerization of Acrylates: Could Microflow Synthesis Make the Difference?. Macromolecular Rapid Communications, 2015, 36, 2149-2155.	2.0	67
84	Carbon capture and utilization in the steel industry: challenges and opportunities for chemical engineering. Current Opinion in Chemical Engineering, 2019, 26, 81-87.	3.8	67
85	Ab Initio Group Contribution Method for Activation Energies of Hydrogen Abstraction Reactions. ChemPhysChem, 2006, 7, 188-199.	1.0	66
86	Physisorption and Chemisorption of Linear Alkenes in Zeolites: A Combined QM-Pot(MP2//B3LYP:GULP)â€“Statistical Thermodynamics Study. Journal of Physical Chemistry C, 2011, 115, 23831-23847.	1.5	66
87	Fe-Containing Magnesium Aluminate Support for Stability and Carbon Control during Methane Reforming. ACS Catalysis, 2018, 8, 5983-5995.	5.5	66
88	The Influence of Dimethyl Disulfide on Naphtha Steam Cracking. Industrial & Engineering Chemistry Research, 2001, 40, 4353-4362.	1.8	65
89	Effect of Clustering on Gasâˆ’Solid Drag in Dilute Two-Phase Flow. Industrial & Engineering Chemistry Research, 2004, 43, 4635-4646.	1.8	65
90	Reaction path analysis for 1-butanol dehydration in H-ZSM-5 zeolite: Ab initio and microkinetic modeling. Journal of Catalysis, 2015, 330, 28-45.	3.1	65

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91	Fed-Batch Control and Visualization of Monomer Sequences of Individual ICAR ATRP Gradient Copolymer Chains. Polymers, 2014, 6, 1074-1095.	2.0	64
92	The total oxidation of propane over supported Cu and Ce oxides: A comparison of single and binary metal oxides. Journal of Catalysis, 2010, 272, 109-120.	3.1	63
93	Kinetics of the oxidative coupling of methane at atmospheric pressure in the absence of catalyst. Industrial & Engineering Chemistry Research, 1991, 30, 2088-2097.	1.8	62
94	Rapeseed oil methyl ester pyrolysis: On-line product analysis using comprehensive two-dimensional gas chromatography. Journal of Chromatography A, 2011, 1218, 3217-3223.	1.8	62
95	MAMA-SG1 initiated nitroxide mediated polymerization of styrene: From Arrhenius parameters to model-based design. Chemical Engineering Journal, 2015, 278, 407-420.	6.6	62
96	Kinetics of a Gas-Phase Chain Reaction Catalyzed by a Solid:Â The Oxidative Coupling of Methane over Li/MgO-Based Catalysts. Industrial & Engineering Chemistry Research, 1996, 35, 3999-4011.	1.8	61
97	Hydrogenation kinetics of toluene on Pt/ZSM-22. Chemical Engineering Journal, 2002, 90, 117-129.	6.6	61
98	Alkylcarbenium Ion Concentrations in Zeolite Pores During Octane Hydrocracking on Pt/H-USY Zeolite. Catalysis Letters, 2004, 94, 81-88.	1.4	61
99	A systematic methodology for kinetic modeling of chemical reactions applied to nâ€hexane hydroisomerization. AIChE Journal, 2015, 61, 880-892.	1.8	61
100	Single-Event Rate Parameters for the Hydrocracking of Cycloalkanes on Pt/US-Y Zeolites. Industrial & Engineering Chemistry Research, 2001, 40, 1832-1844.	1.8	60
101	Group Additive Values for the Gasâ€Phase Standard Enthalpy of Formation, Entropy and Heat Capacity of Oxygenates. Chemistry - A European Journal, 2013, 19, 16431-16452.	1.7	60
102	Catalytic Fast Pyrolysis of Pine Wood: Effect of Successive Catalyst Regeneration. Energy & Fuels, 2014, 28, 4560-4572.	2.5	60
103	CO2 conversion to CO by auto-thermal catalyst-assisted chemical looping. Journal of CO2 Utilization, 2016, 16, 8-16.	3.3	60
104	Methane aromatisation based upon elementary steps: Kinetic and catalyst descriptors. Microporous and Mesoporous Materials, 2012, 164, 302-312.	2.2	59
105	Spatial arrangement and acid strength effects on acidâ€“base cooperatively catalyzed aldol condensation on aminosilica materials. Journal of Catalysis, 2015, 325, 19-25.	3.1	59
106	Coke Formation in the Transfer Line Exchanger during Steam Cracking of Hydrocarbons. Industrial & Engineering Chemistry Research, 2009, 48, 10343-10358.	1.8	58
107	Influence of the Reactor Material Composition on Coke Formation during Ethane Steam Cracking. Industrial & Engineering Chemistry Research, 2014, 53, 6358-6371.	1.8	58
108	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. Combustion and Flame, 2018, 187, 247-256.	2.8	58

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109	A multi-layered view of chemical and biochemical engineering. Chemical Engineering Research and Design, 2020, 155, A133-A145.	2.7	58
110	The conversion of methanol to olefins: a transient kinetic study. Chemical Engineering Science, 1999, 54, 4385-4395.	1.9	57
111	Theoretical Study of the Thermal Decomposition of Dimethyl Disulfide. Journal of Physical Chemistry A, 2010, 114, 10531-10549.	1.1	57
112	The Long and the Short of Radical Polymerization. Macromolecules, 2015, 48, 492-501.	2.2	57
113	Deactivation Study of Fe₂O₃â€“CeO₂ during Redox Cycles for CO Production from CO₂. Industrial & Engineering Chemistry Research, 2016, 55, 5911-5922.	1.8	56
114	State-of-the-art of Coke Formation during Steam Cracking: Anti-Coking Surface Technologies. Industrial & Engineering Chemistry Research, 2018, 57, 16117-16136.	1.8	56
115	Three-dimensional flow patterns in cracking furnaces with long-flame burners. AIChE Journal, 2001, 47, 388-400.	1.8	55
116	Physisorption and Chemisorption of Hydrocarbons in H-FAU Using QM-Pot(MP2//B3LYP) Calculations. Journal of Physical Chemistry C, 2008, 112, 11796-11812.	1.5	55
117	Kinetic Monte Carlo Modeling of the Sulfinyl Precursor Route for Poly(p-phenylene vinylene) Synthesis. Macromolecules, 2011, 44, 8716-8726.	2.2	55
118	An Experimental and Kinetic Modeling Study of Pyrolysis and Combustion of Acetoneâ€“Butanolâ€“Ethanol (ABE) Mixtures. Combustion Science and Technology, 2012, 184, 942-955.	1.2	55
119	Pt/H-ZSM-22 hydroisomerization catalysts optimization guided by Single-Event MicroKinetic modeling. Journal of Catalysis, 2012, 290, 165-176.	3.1	55
120	Sustainable innovations in steam cracking: CO₂ neutral olefin production. Reaction Chemistry and Engineering, 2020, 5, 239-257.	1.9	55
121	Kinetic Monte Carlo Modeling Extracts Information on Chain Initiation and Termination from Complete PLP-SEC Traces. Macromolecules, 2017, 50, 1371-1385.	2.2	54
122	An Update on the Pivotal Role of Kinetic Modeling for the Mechanistic Understanding and Design of Bulk and Solution RAFT Polymerization. Macromolecular Theory and Simulations, 2017, 26, 1600048.	0.6	54
123	Artificial Intelligence in Steam Cracking Modeling: A Deep Learning Algorithm for Detailed Effluent Prediction. Engineering, 2019, 5, 1027-1040.	3.2	54
124	Three-Dimensional Simulation of a Fluid Catalytic Cracking Riser Reactor. Industrial & Engineering Chemistry Research, 2003, 42, 2602-2617.	1.8	53
125	Design and cold flow testing of a Gas-Solid Vortex Reactor demonstration unit for biomass fast pyrolysis. Chemical Engineering Journal, 2017, 329, 198-210.	6.6	53
126	The role of mass and heat transfer in the design of novel reactors for oxidative coupling of methane. Chemical Engineering Science, 2019, 198, 268-289.	1.9	53

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127	Single-Event Microkinetic Model for Fischerâ"Tropsch Synthesis on Iron-Based Catalysts. Industrial & Engineering Chemistry Research, 2008, 47, 5879-5891.	1.8	52
128	Insights into the Reaction Mechanism of Ethanol Conversion into Hydrocarbons on Hâ€ZSMâ€5. Angewandte Chemie - International Edition, 2016, 55, 12817-12821.	7.2	52
129	A comprehensive kinetic model for Cu catalyzed liquid phase glycerol hydrogenolysis. Applied Catalysis B: Environmental, 2017, 205, 469-480.	10.8	52
130	Rotating fluidized bed with a static geometry: Guidelines for design and operating conditions. Chemical Engineering Science, 2010, 65, 1678-1693.	1.9	51
131	Modeling the influence of resonance stabilization on the kinetics of hydrogen abstractions. Physical Chemistry Chemical Physics, 2010, 12, 1278-1298.	1.3	51
132	Model-Based Design To Push the Boundaries of Sequence Control. Macromolecules, 2016, 49, 9336-9344.	2.2	51
133	Irreducible Mass-Transport Limitations during a Heterogeneously Catalyzed Gas-Phase Chain Reaction:Â Oxidative Coupling of Methane. Industrial & Engineering Chemistry Research, 1996, 35, 415-421.	1.8	50
134	TiO2 films prepared by DC magnetron sputtering from ceramic targets. Vacuum, 2002, 68, 31-38.	1.6	50
135	Hydrogen Radical Additions to Unsaturated Hydrocarbons and the Reverse Î²â€Scission Reactions: Modeling of Activation Energies and Preâ€Exponential Factors. ChemPhysChem, 2010, 11, 195-210.	1.0	50
136	Molecular reconstruction of complex hydrocarbon mixtures: An application of principal component analysis. AICHE Journal, 2010, 56, 3174-3188.	1.8	50
137	Influence of Silicon and Silicon/Sulfur-Containing Additives on Coke Formation during Steam Cracking of Hydrocarbons. Industrial & Engineering Chemistry Research, 2008, 47, 1468-1482.	1.8	49
138	Atom Transfer Radical Polymerization of Isobornyl Acrylate: A Kinetic Modeling Study. Macromolecules, 2010, 43, 8766-8781.	2.2	49
139	Kinetic Modeling as a Tool to Understand and Improve the Nitroxide Mediated Polymerization of Styrene. Macromolecular Theory and Simulations, 2011, 20, 238-265.	0.6	49
140	Computational fluid dynamicsâ€based design of finned steam cracking reactors. AICHE Journal, 2014, 60, 794-808.	1.8	48
141	Silanolâ€Assisted Aldol Condensation on Aminated Silica: Understanding the Arrangement of Functional Groups. ChemCatChem, 2014, 6, 255-264.	1.8	48
142	Experimental and Modeling Study on the Thermal Decomposition of Jet Propellant-10. Energy & Fuels, 2014, 28, 4976-4985.	2.5	48
143	Swirl flow tube reactor technology: An experimental and computational fluid dynamics study. Chemical Engineering Journal, 2014, 238, 56-65.	6.6	48
144	CFD-based design of 3D pyrolysis reactors: RANS vs. LES. Chemical Engineering Journal, 2015, 282, 66-76.	6.6	48

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145	Catalyst-assisted chemical looping auto-thermal dry reforming: Spatial structuring effects on process efficiency. Applied Catalysis B: Environmental, 2018, 231, 123-136.	10.8	48
146	Estimation of intrinsic rate coefficients in vinyl chloride suspension polymerization. Polymer, 2005, 46, 8340-8354.	1.8	47
147	Dimensional analysis for scaling up and down steam cracking coils. Chemical Engineering Journal, 2007, 134, 3-10.	6.6	47
148	Effects of amine structure and base strength on acidâ€“base cooperative aldol condensation. Catalysis Today, 2015, 246, 35-45.	2.2	47
149	Oxidative Coupling of Methane: A Microkinetic Model Accounting for Intraparticle Surface-Intermediates Concentration Profiles. Industrial & Engineering Chemistry Research, 2014, 53, 1825-1840.	1.8	46
150	Kinetic Modeling of Jet Propellant-10 Pyrolysis. Energy & Fuels, 2015, 29, 413-427.	2.5	46
151	Hydrocarbon Bond Dissociation Enthalpies: From Substituted Aromatics to Large Polyaromatics. ChemPhysChem, 2006, 7, 2205-2214.	1.0	45
152	Theoretical Study of the Adsorption of the Butanol Isomers in H-ZSM-5. Journal of Physical Chemistry C, 2011, 115, 8658-8669.	1.5	45
153	Catalytic Coating for Reduced Coke Formation in Steam Cracking Reactors. Industrial & Engineering Chemistry Research, 2015, 54, 9525-9535.	1.8	45
154	Hydrogen and Carbon Monoxide Production by Chemical Looping over Ironâ€Aluminium Oxides. Energy Technology, 2016, 4, 304-313.	1.8	45
155	Kinetic Monte Carlo Generation of Complete Electron Spray Ionization Mass Spectra for Acrylate Macromonomer Synthesis. Macromolecules, 2017, 50, 2625-2636.	2.2	45
156	Modeling the Gasâ€Phase Thermochemistry of Organosulfur Compounds. Chemistry - A European Journal, 2011, 17, 7656-7673.	1.7	44
157	Isobutene Protonation in H-FAU, H-MOR, H-ZSM-5, and H-ZSM-22. Journal of Physical Chemistry C, 2012, 116, 18236-18249.	1.5	44
158	First-Principles Kinetic Study on the Effect of the Zeolite Framework on 1-Butanol Dehydration. ACS Catalysis, 2016, 6, 4081-4094.	5.5	44
159	Atomic Layer Deposition Route To Tailor Nanoalloys of Noble and Non-noble Metals. ACS Nano, 2016, 10, 8770-8777.	7.3	44
160	Particle by Particle Kinetic Monte Carlo Tracking of Reaction and Mass Transfer Events in Miniemulsion Free Radical Polymerization. Macromolecules, 2019, 52, 1408-1423.	2.2	44
161	The effects of abrupt T-outlets in a riser: 3D simulation using the kinetic theory of granular flow. Chemical Engineering Science, 2003, 58, 877-885.	1.9	43
162	Modeling the reaction event history and microstructure of individual macrospecies in postpolymerization modification. AICHE Journal, 2017, 63, 4944-4961.	1.8	43

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163	Skeletal isomerization of octadecane on bifunctional ZSM-23 zeolite catalyst. Catalysis Letters, 2005, 100, 235-242.	1.4	42
164	A Theoretical Exploration of the Potential of ICAR ATRP for Oneâ€•and Twoâ€Pot Synthesis of Wellâ€Ðefined Diblock Copolymers. Macromolecular Reaction Engineering, 2013, 7, 311-326.	0.9	42
165	Effect of Rh in Ni-based catalysts on sulfur impurities during methane reforming. Applied Catalysis B: Environmental, 2020, 267, 118691.	10.8	42
166	Two Severity Indices for Scale-Up of Steam Cracking Coils. Industrial & Engineering Chemistry Research, 2005, 44, 3402-3411.	1.8	41
167	Thermochemistry and Kinetics of Hydrogen Abstraction by Methyl Radical from Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2006, 110, 13624-13631.	1.1	41
168	In-situ XAS study on the Cu and Ce local structural changes in a CuOâ€“CeO2/Al2O3 catalyst under propane reduction and re-oxidation. Journal of Physics and Chemistry of Solids, 2009, 70, 1274-1284.	1.9	41
169	Theoretical Study of the Effect of (001) TiO₂Anatase Support on V₂O₅. Journal of Physical Chemistry C, 2010, 114, 3115-3130.	1.5	41
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