Guy B Marin

List of Publications by Citations

496 papers	17,259 citations	64 h-index	99 g-index
514 ext. papers	19,547 ext. citations	6 avg, IF	7.04 L-index

#	Paper	IF	Citations
496	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	1.7	1096
495	New Trends in Olefin Production. *Engineering*, **2017**, 3, 171-178	9.7	320
494	Enhanced Carbon-Resistant Dry Reforming Fe-Ni Catalyst: Role of Fe. *ACS Catalysis*, **2015**, 5, 3028-3039	13.1	283
493	Super-dry reforming of methane intensifies CO2 utilization via Le Chatelier's principle. *Science*, **2016**, 354, 449-452	33.3	240
492	Comprehensive reaction mechanism for n-butanol pyrolysis and combustion. *Combustion and Flame* , **2011**, 158, 16-41	5.3	210
491	Simulation of heterogeneously MgO-catalyzed transesterification for fine-chemical and biodiesel industrial production. *Applied Catalysis B: Environmental*, **2006**, 67, 136-148	21.8	193
490	Kinetics of heterogeneously MgO-catalyzed transesterification. *Applied Catalysis B: Environmental*, **2006**, 62, 35-45	21.8	168
489	Adsorption of C2□8 n-Alkanes in Zeolites□ *Journal of Physical Chemistry C*, **2011**, 115, 1204-1219	3.8	165
488	Modeling the evaporation of a hydrocarbon feedstock in the convection section of a steam cracker. *Computers and Chemical Engineering*, **2009**, 33, 122-132	4	151
487	Ab Initio Calculations for Hydrocarbons: Enthalpy of Formation, Transition State Geometry, and Activation Energy for Radical Reactions. *Journal of Physical Chemistry A*, **2003**, 107, 9147-9159	2.8	150
486	Density Functional Study of Benzene Adsorption on Pt(111). *Journal of Physical Chemistry B*, **2002**, 106, 7489-7498	3.4	147
485	The strength of multi-scale modeling to unveil the complexity of radical polymerization. *Progress in Polymer Science*, **2016**, 58, 59-89	29.6	137
484	Zeolite shape-selectivity in the gem-methylation of aromatic hydrocarbons. *Angewandte Chemie - International Edition*, **2007**, 46, 1311-4	16.4	135
483	First principle kinetic studies of zeolite-catalyzed methylation reactions. *Journal of the American Chemical Society*, **2011**, 133, 888-99	16.4	133
482	The Chemical Route to a Carbon Dioxide Neutral World. *ChemSusChem*, **2017**, 10, 1039-1055	8.3	129
481	Carbon gasification from Fe□Ni catalysts after methane dry reforming. *Applied Catalysis B: Environmental*, **2016**, 185, 42-55	21.8	127
480	Microkinetics of methane oxidative coupling. *Catalysis Today*, **2008**, 137, 90-102	5.3	123

479	Linear Gradient Quality of ATRP Copolymers. *Macromolecules*, **2012**, 45, 8519-8531	5.5	120
478	CeO2-Modified Fe2O3 for CO2 Utilization via Chemical Looping. *Industrial & Engineering Chemistry Research*, **2013**, 52, 8416-8426	3.9	119
477	Theoretical study of the thermodynamics and kinetics of hydrogen abstractions from hydrocarbons. *Journal of Physical Chemistry A*, **2007**, 111, 11771-86	2.8	117
476	Theoretical insights on methylbenzene side-chain growth in ZSM-5 zeolites for methanol-to-olefin conversion. *Chemistry - A European Journal*, **2009**, 15, 10803-8	4.8	114
475	Acid□Metal Balance of a Hydrocracking Catalyst: Ideal versus Nonideal Behavior. *Industrial & Engineering Chemistry Research*, **2005**, 44, 5159-5169	3.9	113
474	Group additive values for the gas phase standard enthalpy of formation of hydrocarbons and hydrocarbon radicals. *Journal of Physical Chemistry A*, **2005**, 109, 7466-80	2.8	113
473	Eurokin. Chemical Reaction Kinetics in Practice. *Cattech*, **2001**, 5, 36-60		103
472	The Crucial Role of Diffusional Limitations in Controlled Radical Polymerization. *Macromolecular Reaction Engineering*, **2013**, 7, 362-379	1.5	100
471	Automatic reaction network generation using RMG for steam cracking of n-hexane. *AICHE Journal*, **2006**, 52, 718-730	3.6	97
470	Catalyst-assisted chemical looping for CO2 conversion to CO. *Applied Catalysis B: Environmental*, **2015**, 164, 184-191	21.8	91
469	Genesys: Kinetic model construction using chemo-informatics. *Chemical Engineering Journal*, **2012**, 207-208, 526-538	14.7	90
468	Physisorption and chemisorption of alkanes and alkenes in H-FAU: a combined ab initio-statistical thermodynamics study. *Physical Chemistry Chemical Physics*, **2009**, 11, 2939-58	3.6	89
467	The Rise and Fall of Direct Mechanisms in Methanol-to-Olefin Catalysis: An Overview of Theoretical Contributions. *Industrial & Engineering Chemistry Research*, **2007**, 46, 8832-8838	3.9	89
466	The coordinatively saturated vanadium MIL-47 as a low leaching heterogeneous catalyst in the oxidation of cyclohexene. *Journal of Catalysis*, **2012**, 285, 196-207	7.3	87
465	Dynamic methods for catalytic kinetics. *Applied Catalysis A: General*, **2008**, 342, 3-28	5.1	86
464	Delivering a Modifying Element to Metal Nanoparticles via Support: Pt□a Alloying during the Reduction of Pt/Mg(Al,Ga)Ox Catalysts and Its Effects on Propane Dehydrogenation. *ACS Catalysis*, **2014**, 4, 1812-1824	13.1	85
463	Normal Mode Analysis in Zeolites: Toward an Efficient Calculation of Adsorption Entropies. *Journal of Chemical Theory and Computation*, **2011**, 7, 1090-101	6.4	85
462	Characterization and Comparison of Fast Pyrolysis Bio-oils from Pinewood, Rapeseed Cake, and Wheat Straw Using C NMR and Comprehensive GC □GC. *ACS Sustainable Chemistry and Engineering*, **2016**, 4, 4974-4985	8.3	84

461	Comprehensive compositional analysis of sulfur and nitrogen containing compounds in shale oil using GC GC FID/SCD/NCD/TOF-MS. *Fuel*, **2015**, 140, 398-406	7.1	83
460	Development of a transient kinetic model for the CO oxidation by O2 over a Pt/Rh/CeO2/Al2O3 three-way catalyst. *Applied Catalysis B: Environmental*, **1998**, 19, 245-259	21.8	82
459	An XPS study on the surface reduction of V2O5(001) induced by Ar+ ion bombardment. *Surface Science*, **2006**, 600, 3512-3517	1.8	81
458	Automatic Mechanism and Kinetic Model Generation for Gas- and Solution-Phase Processes: A Perspective on Best Practices, Recent Advances, and Future Challenges. *International Journal of Chemical Kinetics*, **2015**, 47, 199-231	1.4	80
457	Low-Temperature Atomic Layer Deposition of Platinum Using (Methylcyclopentadienyl)trimethylplatinum and Ozone. *Journal of Physical Chemistry C*, **2013**, 117, 20557-20561	4.8	80
456	ARGET ATRP of Butyl Methacrylate: Utilizing Kinetic Modeling To Understand Experimental Trends. *Macromolecules*, **2013**, 46, 3828-3840	5.5	79
455	Model-based design of the polymer microstructure: bridging the gap between polymer chemistry and engineering. *Polymer Chemistry*, **2015**, 6, 7081-7096	4.9	78
454	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	5.5	78
453	On-line analysis of complex hydrocarbon mixtures using comprehensive two-dimensional gas chromatography. *Journal of Chromatography A*, **2010**, 1217, 6623-33	4.5	78
452	Carbon-centered radical addition and beta-scission reactions: modeling of activation energies and pre-exponential factors. *ChemPhysChem*, **2008**, 9, 124-40	3.2	78
451	Kinetic Modeling of ICAR ATRP. *Macromolecular Theory and Simulations*, **2012**, 21, 52-69	1.5	77
450	Ab initio group contribution method for activation energies for radical additions. *AICHE Journal*, **2004**, 50, 426-444	3.6	77
449	Reaction network for the total oxidation of toluene over CuOCeO2/Al2O3. *Journal of Catalysis*, **2011**, 283, 1-9	7.3	76
448	Methodology for Kinetic Modeling of Atom Transfer Radical Polymerization. *Macromolecular Reaction Engineering*, **2009**, 3, 185-209	1.5	76
447	Catalyst design based on microkinetic models: Oxidative coupling of methane. *Catalysis Today*, **2011**, 159, 29-36	5.3	75
446	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, 12235-51	2.8	75
445	Modeling fast biomass pyrolysis in a gassolid vortex reactor. *Chemical Engineering Journal*, **2012**, 207-208, 195-208	14.7	74
444	Ethanol to higher hydrocarbons over Ni, Ga, Fe-modified ZSM-5: Effect of metal content. *Applied Catalysis A: General*, **2015**, 492, 117-126	5.1	70

443	Nature of the active sites for the total oxidation of toluene by CuOCeO2/Al2O3. *Journal of Catalysis*, **2012**, 295, 91-103	7.3	70
442	Molecular reconstruction of naphtha steam cracking feedstocks based on commercial indices. *Computers and Chemical Engineering*, **2007**, 31, 1020-1034	4	70
441	Single-Event Microkinetics for Methanol to Olefins on H-ZSM-5. *Industrial & Engineering Chemistry Research*, **2013**, 52, 1491-1507	3.9	69
440	Accurate High-Temperature Reaction Networks for Alternative Fuels: Butanol Isomers. *Industrial & Engineering Chemistry Research*, **2010**, 49, 10399-10420	3.9	68
439	Kinetic Modeling of Radical Thiol-Ene Chemistry for Macromolecular Design: Importance of Side Reactions and Diffusional Limitations. *Macromolecules*, **2013**, 46, 1732-1742	5.5	67
438	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	3.4	67
437	An experimental and kinetic modeling study of cyclopentadiene pyrolysis: First growth of polycyclic aromatic hydrocarbons. *Combustion and Flame*, **2014**, 161, 2739-2751	5.3	66
436	The thermal decomposition of 2,5-dimethylfuran. *Proceedings of the Combustion Institute*, **2013**, 34, 251-258	3.9	66
435	Controlling the stability of a Fe-Ni reforming catalyst: Structural organization of the active components. *Applied Catalysis B: Environmental*, **2017**, 209, 405-416	21.8	65
434	Density Functional Theory Analysis of Benzene (De)hydrogenation on Pt(111): Addition and Removal of the First Two H-Atoms. *Journal of Physical Chemistry B*, **2003**, 107, 3844-3855	3.4	65
433	Upgrading the value of anaerobic digestion via chemical production from grid injected biomethane. *Energy and Environmental Science*, **2018**, 11, 1788-1802	35.4	64
432	Formation of ZSM-22 zeolite catalytic particles by fusion of elementary nanorods. *Chemistry - A European Journal*, **2007**, 13, 10070-7	4.8	64
431	The Positive Role of Hydrogen on the Dehydrogenation of Propane on Pt(111). *ACS Catalysis*, **2017**, 7, 7495-7508	13.1	62
430	Improved Livingness and Control over Branching in RAFT Polymerization of Acrylates: Could Microflow Synthesis Make the Difference?. *Macromolecular Rapid Communications*, **2015**, 36, 2149-55	4.8	62
429	Theoretical study of the adsorption of C1-C4 primary alcohols in H-ZSM-5. *Physical Chemistry Chemical Physics*, **2010**, 12, 9481-93	3.6	62
428	Influence of Dimethyl Disulfide on Coke Formation during Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2007**, 46, 4134-4148	3.9	62
427	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	3.8	62
426	Reaction path analysis of propane selective oxidation over V2O5 and V2O5/TiO2. *Journal of Catalysis*, **2012**, 289, 127-139	7.3	61

425	Ab initio thermochemistry and kinetics for carbon-centered radical addition and beta-scission reactions. *Journal of Physical Chemistry A*, **2007**, 111, 8416-28	2.8	61
424	Ab initio group contribution method for activation energies of hydrogen abstraction reactions. *ChemPhysChem*, **2006**, 7, 188-99	3.2	61
423	Effect of Clustering on Gas□Solid Drag in Dilute Two-Phase Flow. *Industrial & Engineering Chemistry Research*, **2004**, 43, 4635-4646	3.9	61
422	The effect of bismuth on the selective oxidation of lactose on supported palladium catalysts. *Carbohydrate Research*, **1990**, 204, 121-9	2.9	60
421	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	7.3	58
420	The Influence of Dimethyl Disulfide on Naphtha Steam Cracking. *Industrial & Engineering Chemistry Research*, **2001**, 40, 4353-4362	3.9	58
419	Biomass to olefins: Cracking of renewable naphtha. *Chemical Engineering Journal*, **2011**, 176-177, 178-187	14.7	57
418	Alkylcarbenium Ion Concentrations in Zeolite Pores During Octane Hydrocracking on Pt/H-USY Zeolite. *Catalysis Letters*, **2004**, 94, 81-88	2.8	57
417	Mg□Fe□Al□O for advanced CO2 to CO conversion: carbon monoxide yield vs. oxygen storage capacity. *Journal of Materials Chemistry A*, **2015**, 3, 16251-16262	13	56
416	Fed-Batch Control and Visualization of Monomer Sequences of Individual ICAR ATRP Gradient Copolymer Chains. *Polymers*, **2014**, 6, 1074-1095	4.5	56
415	Hydrogenation kinetics of toluene on Pt/ZSM-22. *Chemical Engineering Journal*, **2002**, 90, 117-129	14.7	56
414	The role of CO2 in the dehydrogenation of propane over WO□/VO□/SiO2. *Journal of Catalysis*, **2016**, 335, 1-10	7.3	55
413	Advanced Chemical Looping Materials for CO□Utilization: A Review. *Materials*, **2018**, 11,	3.5	54
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411	Catalytic Fast Pyrolysis of Pine Wood: Effect of Successive Catalyst Regeneration. *Energy & Fuels*, **2014**, 28, 4560-4572	4.1	53
410	Physisorption and Chemisorption of Linear Alkenes in Zeolites: A Combined QM-Pot(MP2//B3LYP:GULP)□Statistical Thermodynamics Study. *Journal of Physical Chemistry C*, **2011**, 115, 23831-23847	3.8	53
409	Single-Event Rate Parameters for the Hydrocracking of Cycloalkanes on Pt/US-Y Zeolites. *Industrial & Engineering Chemistry Research*, **2001**, 40, 1832-1844	3.9	52
408	DFT-based microkinetic modeling of ethanol dehydration in H-ZSM-5. *Journal of Catalysis*, **2016**, 339, 173-185	7.3	52

407	Fe-Containing Magnesium Aluminate Support for Stability and Carbon Control during Methane Reforming. *ACS Catalysis*, **2018**, 8, 5983-5995	13.1	52
406	Reaction path analysis for 1-butanol dehydration in H-ZSM-5 zeolite: Ab initio and microkinetic modeling. *Journal of Catalysis*, **2015**, 330, 28-45	7.3	51
405	Experimental and modeling study of the pyrolysis and combustion of dimethoxymethane. *Combustion and Flame*, **2018**, 190, 270-283	5.3	51
404	An Experimental and Kinetic Modeling Study of Pyrolysis and Combustion of AcetoneButanolEthanol (ABE) Mixtures. *Combustion Science and Technology*, **2012**, 184, 942-955	1.5	51
403	First principle-based simulation of ethane steam cracking. *AICHE Journal*, **2011**, 57, 482-496	3.6	51
402	Kinetic modeling of the total oxidation of propane over CuO-CeO2/Al2O3. *Applied Catalysis B: Environmental*, **2010**, 95, 26-38	21.8	51
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400	Spatial arrangement and acid strength effects on acidBase cooperatively catalyzed aldol condensation on aminosilica materials. *Journal of Catalysis*, **2015**, 325, 19-25	7.3	50
399	Methane aromatisation based upon elementary steps: Kinetic and catalyst descriptors. *Microporous and Mesoporous Materials*, **2012**, 164, 302-312	5.3	50
398	Theoretical study of the thermal decomposition of dimethyl disulfide. *Journal of Physical Chemistry A*, **2010**, 114, 10531-49	2.8	50
397	Kinetic Monte Carlo Modeling of the Sulfinyl Precursor Route for Poly(p-phenylene vinylene) Synthesis. *Macromolecules*, **2011**, 44, 8716-8726	5.5	50
396	Three-dimensional flow patterns in cracking furnaces with long-flame burners. *AICHE Journal*, **2001**, 47, 388-400	3.6	50
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394	Coke Formation in the Transfer Line Exchanger during Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2009**, 48, 10343-10358	3.9	49
393	Kinetics of the oxidative coupling of methane at atmospheric pressure in the absence of catalyst. *Industrial & Engineering Chemistry Research*, **1991**, 30, 2088-2097	3.9	49
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391	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	1.5	48
390	The Long and the Short of Radical Polymerization. *Macromolecules*, **2015**, 48, 492-501	5.5	48

389	The conversion of methanol to olefins: a transient kinetic study. *Chemical Engineering Science*, **1999**, 54, 4385-4395	4.4	48
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387	MAMA-SG1 initiated nitroxide mediated polymerization of styrene: From Arrhenius parameters to model-based design. *Chemical Engineering Journal*, **2015**, 278, 407-420	14.7	47
386	Rapeseed oil methyl ester pyrolysis: on-line product analysis using comprehensive two-dimensional gas chromatography. *Journal of Chromatography A*, **2011**, 1218, 3217-23	4.5	47
385	Single-Event Microkinetic Model for Fischer□Tropsch Synthesis on Iron-Based Catalysts. *Industrial & Engineering Chemistry Research*, **2008**, 47, 5879-5891	3.9	47
384	A systematic methodology for kinetic modeling of chemical reactions applied to n-hexane hydroisomerization. *AICHE Journal*, **2015**, 61, 880-892	3.6	46
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382	Modeling the influence of resonance stabilization on the kinetics of hydrogen abstractions. *Physical Chemistry Chemical Physics*, **2010**, 12, 1278-98	3.6	46
381	Three-Dimensional Simulation of a Fluid Catalytic Cracking Riser Reactor. *Industrial & Engineering Chemistry Research*, **2003**, 42, 2602-2617	3.9	46
380	Kinetic Modeling as a Tool to Understand and Improve the Nitroxide Mediated Polymerization of Styrene. *Macromolecular Theory and Simulations*, **2011**, 20, 238-265	1.5	45
379	Atom Transfer Radical Polymerization of Isobornyl Acrylate: A Kinetic Modeling Study. *Macromolecules*, **2010**, 43, 8766-8781	5.5	45
378	Hydrocarbon bond dissociation enthalpies: from substituted aromatics to large polyaromatics. *ChemPhysChem*, **2006**, 7, 2205-14	3.2	45
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376	Model-Based Design To Push the Boundaries of Sequence Control. *Macromolecules*, **2016**, 49, 9336-9344	5.5	45
375	Rotating fluidized bed with a static geometry: Guidelines for design and operating conditions. *Chemical Engineering Science*, **2010**, 65, 1678-1693	4.4	44
374	Hydrogen radical additions to unsaturated hydrocarbons and the reverse beta-scission reactions: modeling of activation energies and pre-exponential factors. *ChemPhysChem*, **2010**, 11, 195-210	3.2	44
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372	A comprehensive kinetic model for Cu catalyzed liquid phase glycerol hydrogenolysis. *Applied Catalysis B: Environmental*, **2017**, 205, 469-480	21.8	43

371	Influence of the Reactor Material Composition on Coke Formation during Ethane Steam Cracking. *Industrial & Engineering Chemistry Research*, **2014**, 53, 6358-6371	3.9	43
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369	Dimensional analysis for scaling up and down steam cracking coils. *Chemical Engineering Journal*, **2007**, 134, 3-10	14.7	43
368	A multi-layered view of chemical and biochemical engineering. *Chemical Engineering Research and Design*, **2020**, 155, A133-A145	5.5	43
367	Pressure dependent kinetic analysis of pathways to naphthalene from cyclopentadienyl recombination. *Combustion and Flame*, **2018**, 187, 247-256	5.3	42
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365	Estimation of intrinsic rate coefficients in vinyl chloride suspension polymerization. *Polymer*, **2005**, 46, 8340-8354	3.9	42
364	Kinetic Monte Carlo Modeling Extracts Information on Chain Initiation and Termination from Complete PLP-SEC Traces. *Macromolecules*, **2017**, 50, 1371-1385	5.5	41
363	Computational fluid dynamics-based design of finned steam cracking reactors. *AICHE Journal*, **2014**, 60, 794-808	3.6	41
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361	Influence of Silicon and Silicon/Sulfur-Containing Additives on Coke Formation during Steam Cracking of Hydrocarbons. *Industrial & Engineering Chemistry Research*, **2008**, 47, 1468-1482	3.9	40
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