Paul H M Van Steenberge

List of Publications by Year
in descending order

89	3,100	136885	189801
papers	citations	32 h-index	50 g-index

89	89	89	1418
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The chemistry of chemical recycling of solid plastic waste via pyrolysis and gasification: State-of-the-art, challenges, and future directions. Progress in Energy and Combustion Science, 2021, 84, 100901.	15.8	297
2	The strength of multi-scale modeling to unveil the complexity of radical polymerization. Progress in Polymer Science, 2016, 58, 59-89.	11.8	174
3	Linear Gradient Quality of ATRP Copolymers. Macromolecules, 2012, 45, 8519-8531.	2.2	139
4	Model-based design of the polymer microstructure: bridging the gap between polymer chemistry and engineering. Polymer Chemistry, 2015, 6, 7081-7096.	1.9	94
5	ARGET ATRP of Butyl Methacrylate: Utilizing Kinetic Modeling To Understand Experimental Trends. Macromolecules, 2013, 46, 3828-3840.	2.2	90
6	Computational prediction of the molecular configuration of three-dimensional network polymers. Nature Materials, 2021, 20, 1422-1430.	13.3	84
7	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
8	Fed-Batch Control and Visualization of Monomer Sequences of Individual ICAR ATRP Gradient Copolymer Chains. Polymers, 2014, 6, 1074-1095.	2.0	64
9	Systematic investigation of alkyl sulfonate initiators for the cationic ring-opening polymerization of 2-oxazolines revealing optimal combinations of monomers and initiators. European Polymer Journal, 2015, 65, 298-304.	2.6	63
10	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
11	Progress in Reaction Mechanisms and Reactor Technologies for Thermochemical Recycling of Poly(methyl methacrylate). Polymers, 2020, 12, 1667.	2.0	62
12	Gillespie-Driven kinetic Monte Carlo Algorithms to Model Events for Bulk or Solution (Bio)Chemical Systems Containing Elemental and Distributed Species. Industrial & Engineering Chemistry Research, 2020, 59, 18357-18386.	1.8	56
13	Kinetic Monte Carlo Modeling of the Sulfinyl Precursor Route for Poly(p-phenylene vinylene) Synthesis. Macromolecules, 2011, 44, 8716-8726.	2.2	55
14	Kinetic Monte Carlo Modeling Extracts Information on Chain Initiation and Termination from Complete PLP-SEC Traces. Macromolecules, 2017, 50, 1371-1385.	2.2	54
15	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
16	Connecting polymer synthesis and chemical recycling on a chain-by-chain basis: a unified matrix-based kinetic Monte Carlo strategy. Reaction Chemistry and Engineering, 2020, 5, 1909-1928.	1.9	53
17	Model-Based Design To Push the Boundaries of Sequence Control. Macromolecules, 2016, 49, 9336-9344.	2.2	51
18	Simulation of the Degradation of Cyclic Ketene Acetal and Vinylâ€Based Copolymers Synthesized via a Radical Process: Influence of the Reactivity Ratios on the Degradability Properties. Macromolecular Rapid Communications, 2018, 39, e1800193.	2.0	47

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19	Visualization and design of the functional group distribution during statistical copolymerization. Nature Communications, 2019, 10, 3641.	5.8	46
20	Kinetic Monte Carlo Generation of Complete Electron Spray Ionization Mass Spectra for Acrylate Macromonomer Synthesis. Macromolecules, 2017, 50, 2625-2636.	2.2	45
21	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
22	Modeling the reaction event history and microstructure of individual macrospecies in postpolymerization modification. AICHE Journal, 2017, 63, 4944-4961.	1.8	43
23	Visibleâ€Lightâ€Induced Passerini Multicomponent Polymerization. Angewandte Chemie - International Edition, 2019, 58, 5672-5676.	7.2	43
24	A Theoretical Exploration of the Potential of ICAR ATRP for Oneâ€•and Twoâ€Pot Synthesis of Wellâ€Defined Diblock Copolymers. Macromolecular Reaction Engineering, 2013, 7, 311-326.	0.9	42
25	4-Dimensional Modeling Strategy for an Improved Understanding of Miniemulsion NMP of Acrylates Initiated by SG1-Macroinitiator. Macromolecules, 2014, 47, 7732-7741.	2.2	41
26	Fusing Light-Induced Step-Growth Processes with RAFT Chemistry for Segmented Copolymer Synthesis: A Synergetic Experimental and Kinetic Modeling Study. Macromolecules, 2017, 50, 6451-6467.	2.2	41
27	A complete understanding of the reaction kinetics for the industrial production process of expandable polystyrene. AICHE Journal, 2017, 63, 2043-2059.	1.8	41
28	From n-butyl acrylate Arrhenius parameters for backbiting and tertiary propagation to Î²-scission via stepwise pulsed laser polymerization. Polymer Chemistry, 2019, 10, 4116-4125.	1.9	38
29	Analytical and advanced kinetic models for characterization of chain-growth copolymerization: the state-of-the-art. Reaction Chemistry and Engineering, 2018, 3, 128-145.	1.9	37
30	How penultimate monomer unit effects and initiator influence ICAR ATRP of nâ€butyl acrylate and methyl methacrylate. AICHE Journal, 2017, 63, 4971-4986.	1.8	35
31	Ab initio based kinetic Monte Carlo analysis to unravel the propagation kinetics in vinyl acetate pulsed laser polymerization. Polymer Chemistry, 2017, 8, 7143-7150.	1.9	35
32	How chain length dependencies interfere with the bulk RAFT polymerization rate and microstructural control. Chemical Engineering Science, 2018, 177, 163-179.	1.9	35
33	Coupled matrix kinetic Monte Carlo simulations applied for advanced understanding of polymer grafting kinetics. Reaction Chemistry and Engineering, 2021, 6, 640-661.	1.9	35
34	ICAR ATRP for Estimation of Intrinsic Macro-Activation/Deactivation Arrhenius Parameters under Polymerization Conditions. Industrial & Engineering Chemistry Research, 2014, 53, 9674-9685.	1.8	33
35	Model-Based Visualization and Understanding of Monomer Sequence Formation in Gradient Copoly(2-oxazoline)s On the basis of 2-Methyl-2-oxazoline and 2-Phenyl-2-oxazoline. Macromolecules, 2015, 48, 7765-7773.	2.2	33
36	Benchmarking Stochastic and Deterministic Kinetic Modeling of Bulk and Solution Radical Polymerization Processes by Including Six Types of Factors Two. Macromolecular Theory and Simulations, 2020, 29, 2000065.	0.6	32

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37	Conformational Distributions near and on the Substrate during Surface-Initiated Living Polymerization: A Lattice-Based Kinetic Monte Carlo Approach. Macromolecules, 2020, 53, 4630-4648.	2.2	32
38	Waterborne Electrospinning of Poly(N-isopropylacrylamide) by Control of Environmental Parameters. ACS Applied Materials & Interfaces, 2017, 9, 24100-24110.	4.0	29
39	Controlled synthesis of poly[(butyl methacrylate)â€coâ€(butyl acrylate)] via activator regenerated by electron transfer atom transfer radical polymerization: insights and improvement. Polymer International, 2014, 63, 848-857.	1.6	27
40	A two-phase stochastic model to describe mass transport and kinetics during reactive processing of polyolefins. Chemical Engineering Journal, 2019, 377, 119980.	6.6	27
41	An alternative method to estimate the bulk backbiting rate coefficient in acrylate radical polymerization. Polymer Chemistry, 2016, 7, 6521-6528.	1.9	26
42	Impact of side reactions on molar mass distribution, unsaturation level and branching density in solution free radical polymerization of n-butyl acrylate under well-defined lab-scale reactor conditions. Polymer Chemistry, 2021, 12, 2095-2114.	1.9	26
43	Access to the Î²-scission rate coefficient in acrylate radical polymerization by careful scanning of pulse laser frequencies at elevated temperature. Reaction Chemistry and Engineering, 2018, 3, 807-815.	1.9	25
44	Exploring the Full Potential of Reversible Deactivation Radical Polymerization Using Pareto-Optimal Fronts. Polymers, 2015, 7, 655-679.	2.0	24
45	Chain Transfer in Degenerative RAFT Polymerization Revisited: A Comparative Study of Literature Methods. Macromolecular Theory and Simulations, 2016, 25, 104-115.	0.6	24
46	Coupled stochastic simulation of the chain length and particle size distribution in miniemulsion radical copolymerization of styrene and N-vinylcaprolactam. Reaction Chemistry and Engineering, 2019, 4, 1935-1947.	1.9	24
47	A detailed mechanistic study of bulk MADIX of styrene and its chain extension. Polymer Chemistry, 2017, 8, 6948-6963.	1.9	23
48	Costâ€efficient modeling of distributed molar mass and topological variations in graft copolymer synthesis by upgrading the method of moments. AICHE Journal, 2022, 68, .	1.8	23
49	Jacket temperature regulation allowing well-defined non-adiabatic lab-scale solution free radical polymerization of acrylates. Reaction Chemistry and Engineering, 2021, 6, 1053-1069.	1.9	22
50	Design of 2â€hydroxyethyl methacrylateâ€functional macromonomer dispersants by semiâ€batch cobalt chain transfer polymerization. AICHE Journal, 2019, 65, e16723.	1.8	21
51	Roadmap for Monomer Conversion and Chain Length-Dependent Termination Reactivity Algorithms in Kinetic Monte Carlo Modeling of Bulk Radical Polymerization. Industrial & Engineering Chemistry Research, 2020, 59, 22422-22439.	1.8	21
52	New Insights in the Treatment of Waste Water with Graphene: Dual-Site Adsorption by Sodium Dodecylbenzenesulfonate. Industrial & Engineering Chemistry Research, 2016, 55, 9387-9396.	1.8	20
53	Estimating the photodissociation quantum yield from PLP-SEC peak heights. Polymer Chemistry, 2017, 8, 3124-3128.	1.9	19
54	Timeâ€Dependent Differential and Integral Quantum Yields for Wavelengthâ€Dependent [4+4] Photocycloadditions. Chemistry - A European Journal, 2020, 26, 478-484.	1.7	19

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55	Translating Simulated Chain Length and Molar Mass Distributions in Chainâ€Growth Polymerization for Experimental Comparison and Mechanistic Insight. Macromolecular Theory and Simulations, 2021, 30, 2100008.	0.6	19
56	Bridging principal component analysis and method of moments based parameter estimation for grafting of polybutadiene with styrene. Chemical Engineering Journal, 2021, 425, 130463.	6.6	19
57	Interplay of Head, Tail, and Mid-Chain Radicals in Bulk Free-Radical and Reversible Degenerative Addition Fragmentation Chain-Transfer Polymerizations of Vinyl Acetate. Macromolecules, 2019, 52, 4555-4569.	2.2	18
58	A kinetic study on the para-fluoro-thiol reaction in view of its use in materials design. Polymer Chemistry, 2019, 10, 2781-2791.	1.9	18
59	Extending Multilevel Statistical Entropy Analysis towards Plastic Recyclability Prediction. Sustainability, 2021, 13, 3553.	1.6	18
60	Connecting Gas-Phase Computational Chemistry to Condensed Phase Kinetic Modeling: The State-of-the-Art. Polymers, 2021, 13, 3027.	2.0	18
61	Synergy of Advanced Experimental and Modeling Tools to Underpin the Synthesis of Static Step-Growth-Based Networks Involving Polymeric Precursor Building Blocks. Macromolecules, 2021, 54, 9280-9298.	2.2	18
62	Multi-scale reactive extrusion modelling approaches to design polymer synthesis, modification and mechanical recycling. Reaction Chemistry and Engineering, 2022, 7, 245-263.	1.9	18
63	Macropropagation Rate Coefficients and Branching Levels in Cationic Ring-Opening Polymerization of 2-Ethyl-2-oxazoline through Prediction of Size Exclusion Chromatography Data. Macromolecules, 2019, 52, 4067-4078.	2.2	17
64	Going Beyond the Carothers, Flory and Stockmayer Equation by Including Cyclization Reactions and Mobility Constraints. Polymers, 2021, 13, 2410.	2.0	17
65	Improved Mechanistic Insights into Radical Sulfinyl Precursor MDMO-PPV Synthesis by Combining Microflow Technology and Computer Simulations. Macromolecules, 2015, 48, 8294-8306.	2.2	16
66	Comparative Kinetic Monte Carlo study of the Sulfinyl and Dithiocarbamate Precursor Route toward Highly Regioregular MDMOâ€PPV. Macromolecular Theory and Simulations, 2013, 22, 246-255.	0.6	15
67	An evaluation of the impact of SG1 disproportionation and the addition of styrene in NMP of methyl methacrylate. AICHE Journal, 2018, 64, 2545-2559.	1.8	15
68	Deterministic Modeling of Degenerative RAFT Miniemulsion Polymerization Rate and Average Polymer Characteristics: Invalidity of Zeroâ€“One Nature at Higher Monomer Conversions. Macromolecules, 2018, 51, 9442-9461.	2.2	14
69	Conformational Variations for Surface-Initiated Reversible Deactivation Radical Polymerization: From Flat to Curved Nanoparticle Surfaces. Macromolecules, 2021, 54, 8270-8288.	2.2	14
70	Sensitivity Analysis of Singleâ€Phase Isothermal Free Radicalâ€“Induced Grafting of Polyethylene. Macromolecular Theory and Simulations, 2018, 27, 1800036.	0.6	13
71	Modeling of Miniemulsion Polymerization of Styrene with Macro-RAFT Agents to Theoretically Compare Slow Fragmentation, Ideal Exchange and Cross-Termination Cases. Polymers, 2019, 11, 320.	2.0	13
72	The Competition of Termination and Shielding to Evaluate the Success of Surface-Initiated Reversible Deactivation Radical Polymerization. Polymers, 2020, 12, 1409.	2.0	13

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73	Distribution Changes during Thermal Degradation of Poly(styrene peroxide) by Pairing Tree-Based Kinetic Monte Carlo and Artificial Intelligence Tools. Industrial & Engineering Chemistry Research, 2021, 60, 3334-3353.	1.8	13
74	Abâ€Initioâ€Based Kinetic Modeling to Understand RAFT Exchange: The Case of 2â€Cyanoâ€2â€Propyl Dodecyl Trithiocarbonate and Styrene. Macromolecular Rapid Communications, 2018, 39, 1700403.	2.0	12
75	A holistic approach for anthracene photochemistry kinetics. Chemical Engineering Journal, 2020, 402, 126259.	6.6	11
76	Sensitivity analysis of isothermal free radical induced grafting through application of the distribution - Numerical fractionation - Method of moments. Chemical Engineering Journal, 2022, 444, 136595.	6.6	11
77	A unified kinetic Monte Carlo approach to evaluate (a)symmetric block and gradient copolymers with linear and branched chains illustrated for poly(2-oxazoline)s. Polymer Chemistry, 2022, 13, 1559-1575.	1.9	10
78	New mechanism for autoxidation of polyolefins: kinetic Monte Carlo modelling of the role of short-chain branches, molecular oxygen and unsaturated moieties. Polymer Chemistry, 2022, 13, 3304-3314.	1.9	9
79	A novel method for the measurement of degenerative chain transfer coefficients: proof of concept and experimental validation. Polymer Chemistry, 2016, 7, 3334-3349.	1.9	8
80	The Relevance of Multiâ€Injection and Temperature Profiles to Design Multiâ€Phase Reactive Processing of Polyolefins. Macromolecular Theory and Simulations, 2019, 28, 1900035.	0.6	8
81	Exploiting (Multicomponent) Semibatch and Jacket Temperature Procedures to Safely Tune Molecular Properties for Solution Free Radical Polymerization of nâ€Butyl Acrylate. Macromolecular Theory and Simulations, 2021, 30, 2100024.	0.6	8
82	Procedures and Guidelines for Inputting and Output Smoothening of Kinetic Monte Carlo Distributions. Advanced Theory and Simulations, 2022, 5, .	1.3	7
83	Exploiting the pulsed laser polymerization-size exclusion chromatography technique to retrieve kinetic parameters in radical polymerization: State-of-the-art and future challenges. Advances in Chemical Engineering, 2020, , 59-95.	0.5	4
84	In Silico Screening To Achieve Fast Lab-Scale Nitroxide-Mediated Polymerization of n-Butyl Acrylate with Maximal Control over Macromolecular Properties. Industrial & Engineering Chemistry Research, 2021, 60, 16981-16992.	1.8	4
85	Differences and similarities between mono-, bi- or tetrafunctional initiated cationic ring-opening polymerization of 2-oxazolines. Polymer Chemistry, 2022, 13, 861-876.	1.9	3
86	Visibleâ€Lightâ€Induced Passerini Multicomponent Polymerization. Angewandte Chemie, 2019, 131, 5728-5732.	1.6	2
87	Green Degradable (Co)Polyacrylics: A Kinetic Monte Carlo Study. , 2020, 69, .		0
88	A Generic Combined Matrix- and Lattice-Based Kinetic Monte Carlo Modeling Tool to Tune Surface-Initiated Polymerization. , 2020, 69, .		0
89	[4+4] Anthracene Photodimerization for Controlled Folding of Single Chain Polymer Nanoparticles. , 2020, 69, .		0