

Paul H M Van Steenberge

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/595361/publications.pdf>

Version: 2024-02-01

89
papers

3,100
citations

136885

32
h-index

189801

50
g-index

89
all docs

89
docs citations

89
times ranked

1418
citing authors

#	ARTICLE	IF	CITATIONS
1	Differences and similarities between mono-, bi- or tetrafunctional initiated cationic ring-opening polymerization of 2-oxazolines. <i>Polymer Chemistry</i> , 2022, 13, 861-876.	1.9	3
2	Multi-scale reactive extrusion modelling approaches to design polymer synthesis, modification and mechanical recycling. <i>Reaction Chemistry and Engineering</i> , 2022, 7, 245-263.	1.9	18
3	Cost-efficient modeling of distributed molar mass and topological variations in graft copolymer synthesis by upgrading the method of moments. <i>AIChE Journal</i> , 2022, 68, .	1.8	23
4	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. <i>Polymer Chemistry</i> , 2022, 13, 1559-1575.	1.9	10
5	New mechanism for autoxidation of polyolefins: kinetic Monte Carlo modelling of the role of short-chain branches, molecular oxygen and unsaturated moieties. <i>Polymer Chemistry</i> , 2022, 13, 3304-3314.	1.9	9
6	Procedures and Guidelines for Inputting and Output Smoothing of Kinetic Monte Carlo Distributions. <i>Advanced Theory and Simulations</i> , 2022, 5, .	1.3	7
7	Sensitivity analysis of isothermal free radical induced grafting through application of the distribution - Numerical fractionation - Method of moments. <i>Chemical Engineering Journal</i> , 2022, 444, 136595.	6.6	11
8	Impact of side reactions on molar mass distribution, unsaturation level and branching density in solution free radical polymerization of <i>n</i> -butyl acrylate under well-defined lab-scale reactor conditions. <i>Polymer Chemistry</i> , 2021, 12, 2095-2114.	1.9	26
9	Jacket temperature regulation allowing well-defined non-adiabatic lab-scale solution free radical polymerization of acrylates. <i>Reaction Chemistry and Engineering</i> , 2021, 6, 1053-1069.	1.9	22
10	Extending Multilevel Statistical Entropy Analysis towards Plastic Recyclability Prediction. <i>Sustainability</i> , 2021, 13, 3553.	1.6	18
11	Translating Simulated Chain Length and Molar Mass Distributions in Chain-Growth Polymerization for Experimental Comparison and Mechanistic Insight. <i>Macromolecular Theory and Simulations</i> , 2021, 30, 2100008.	0.6	19
12	The chemistry of chemical recycling of solid plastic waste via pyrolysis and gasification: State-of-the-art, challenges, and future directions. <i>Progress in Energy and Combustion Science</i> , 2021, 84, 100901.	15.8	297
13	Exploiting (Multicomponent) Semibatch and Jacket Temperature Procedures to Safely Tune Molecular Properties for Solution Free Radical Polymerization of <i>n</i> -Butyl Acrylate. <i>Macromolecular Theory and Simulations</i> , 2021, 30, 2100024.	0.6	8
14	Computational prediction of the molecular configuration of three-dimensional network polymers. <i>Nature Materials</i> , 2021, 20, 1422-1430.	13.3	84
15	Going Beyond the Carothers, Flory and Stockmayer Equation by Including Cyclization Reactions and Mobility Constraints. <i>Polymers</i> , 2021, 13, 2410.	2.0	17
16	Connecting Gas-Phase Computational Chemistry to Condensed Phase Kinetic Modeling: The State-of-the-Art. <i>Polymers</i> , 2021, 13, 3027.	2.0	18
17	Conformational Variations for Surface-Initiated Reversible Deactivation Radical Polymerization: From Flat to Curved Nanoparticle Surfaces. <i>Macromolecules</i> , 2021, 54, 8270-8288.	2.2	14
18	Bridging principal component analysis and method of moments based parameter estimation for grafting of polybutadiene with styrene. <i>Chemical Engineering Journal</i> , 2021, 425, 130463.	6.6	19

#	ARTICLE	IF	CITATIONS
19	Coupled matrix kinetic Monte Carlo simulations applied for advanced understanding of polymer grafting kinetics. <i>Reaction Chemistry and Engineering</i> , 2021, 6, 640-661.	1.9	35
20	Distribution Changes during Thermal Degradation of Poly(styrene peroxide) by Pairing Tree-Based Kinetic Monte Carlo and Artificial Intelligence Tools. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 3334-3353.	1.8	13
21	Synergy of Advanced Experimental and Modeling Tools to Underpin the Synthesis of Static Step-Growth-Based Networks Involving Polymeric Precursor Building Blocks. <i>Macromolecules</i> , 2021, 54, 9280-9298.	2.2	18
22	In Silico Screening To Achieve Fast Lab-Scale Nitroxide-Mediated Polymerization of <i>n</i> -Butyl Acrylate with Maximal Control over Macromolecular Properties. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 16981-16992.	1.8	4
23	Time-Dependent Differential and Integral Quantum Yields for Wavelength-Dependent [4+4] Photocycloadditions. <i>Chemistry - A European Journal</i> , 2020, 26, 478-484.	1.7	19
24	Gillespie-Driven kinetic Monte Carlo Algorithms to Model Events for Bulk or Solution (Bio)Chemical Systems Containing Elemental and Distributed Species. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 18357-18386.	1.8	56
25	A holistic approach for anthracene photochemistry kinetics. <i>Chemical Engineering Journal</i> , 2020, 402, 126259.	6.6	11
26	The Competition of Termination and Shielding to Evaluate the Success of Surface-Initiated Reversible Deactivation Radical Polymerization. <i>Polymers</i> , 2020, 12, 1409.	2.0	13
27	Progress in Reaction Mechanisms and Reactor Technologies for Thermochemical Recycling of Poly(methyl methacrylate). <i>Polymers</i> , 2020, 12, 1667.	2.0	62
28	Connecting polymer synthesis and chemical recycling on a chain-by-chain basis: a unified matrix-based kinetic Monte Carlo strategy. <i>Reaction Chemistry and Engineering</i> , 2020, 5, 1909-1928.	1.9	53
29	Benchmarking Stochastic and Deterministic Kinetic Modeling of Bulk and Solution Radical Polymerization Processes by Including Six Types of Factors Two. <i>Macromolecular Theory and Simulations</i> , 2020, 29, 2000065.	0.6	32
30	Roadmap for Monomer Conversion and Chain Length-Dependent Termination Reactivity Algorithms in Kinetic Monte Carlo Modeling of Bulk Radical Polymerization. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 22422-22439.	1.8	21
31	Exploiting the pulsed laser polymerization-size exclusion chromatography technique to retrieve kinetic parameters in radical polymerization: State-of-the-art and future challenges. <i>Advances in Chemical Engineering</i> , 2020, , 59-95.	0.5	4
32	Conformational Distributions near and on the Substrate during Surface-Initiated Living Polymerization: A Lattice-Based Kinetic Monte Carlo Approach. <i>Macromolecules</i> , 2020, 53, 4630-4648.	2.2	32
33	Green Degradable (Co)Polyacrylics: A Kinetic Monte Carlo Study. , 2020, 69, .		0
34	A Generic Combined Matrix- and Lattice-Based Kinetic Monte Carlo Modeling Tool to Tune Surface-Initiated Polymerization. , 2020, 69, .		0
35	[4+4] Anthracene Photodimerization for Controlled Folding of Single Chain Polymer Nanoparticles. , 2020, 69, .		0
36	Visualization and design of the functional group distribution during statistical copolymerization. <i>Nature Communications</i> , 2019, 10, 3641.	5.8	46

#	ARTICLE	IF	CITATIONS
37	Coupled stochastic simulation of the chain length and particle size distribution in miniemulsion radical copolymerization of styrene and <i>N</i> -vinylcaprolactam. <i>Reaction Chemistry and Engineering</i> , 2019, 4, 1935-1947.	1.9	24
38	Design of 2-hydroxyethyl methacrylate-functional macromonomer dispersants by semi-batch cobalt chain transfer polymerization. <i>AIChE Journal</i> , 2019, 65, e16723.	1.8	21
39	From <i>n</i> -butyl acrylate Arrhenius parameters for backbiting and tertiary propagation to β -scission via stepwise pulsed laser polymerization. <i>Polymer Chemistry</i> , 2019, 10, 4116-4125.	1.9	38
40	The Relevance of Multi-Phase Injection and Temperature Profiles to Design Multi-Phase Reactive Processing of Polyolefins. <i>Macromolecular Theory and Simulations</i> , 2019, 28, 1900035.	0.6	8
41	Particle by Particle Kinetic Monte Carlo Tracking of Reaction and Mass Transfer Events in Miniemulsion Free Radical Polymerization. <i>Macromolecules</i> , 2019, 52, 1408-1423.	2.2	44
42	Macropropagation Rate Coefficients and Branching Levels in Cationic Ring-Opening Polymerization of 2-Ethyl-2-oxazoline through Prediction of Size Exclusion Chromatography Data. <i>Macromolecules</i> , 2019, 52, 4067-4078.	2.2	17
43	Interplay of Head, Tail, and Mid-Chain Radicals in Bulk Free-Radical and Reversible Degenerative Addition Fragmentation Chain-Transfer Polymerizations of Vinyl Acetate. <i>Macromolecules</i> , 2019, 52, 4555-4569.	2.2	18
44	A kinetic study on the <i>para</i> -fluoro-thiol reaction in view of its use in materials design. <i>Polymer Chemistry</i> , 2019, 10, 2781-2791.	1.9	18
45	Visible-Light-Induced Passerini Multicomponent Polymerization. <i>Angewandte Chemie</i> , 2019, 131, 5728-5732.	1.6	2
46	Modeling of Miniemulsion Polymerization of Styrene with Macro-RAFT Agents to Theoretically Compare Slow Fragmentation, Ideal Exchange and Cross-Termination Cases. <i>Polymers</i> , 2019, 11, 320.	2.0	13
47	Visible-Light-Induced Passerini Multicomponent Polymerization. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5672-5676.	7.2	43
48	A two-phase stochastic model to describe mass transport and kinetics during reactive processing of polyolefins. <i>Chemical Engineering Journal</i> , 2019, 377, 119980.	6.6	27
49	Analytical and advanced kinetic models for characterization of chain-growth copolymerization: the state-of-the-art. <i>Reaction Chemistry and Engineering</i> , 2018, 3, 128-145.	1.9	37
50	Ab-Initio-Based Kinetic Modeling to Understand RAFT Exchange: The Case of 2-Cyano-2-Propyl Dodecyl Trithiocarbonate and Styrene. <i>Macromolecular Rapid Communications</i> , 2018, 39, 1700403.	2.0	12
51	How chain length dependencies interfere with the bulk RAFT polymerization rate and microstructural control. <i>Chemical Engineering Science</i> , 2018, 177, 163-179.	1.9	35
52	Deterministic Modeling of Degenerative RAFT Miniemulsion Polymerization Rate and Average Polymer Characteristics: Invalidity of Zero-One Nature at Higher Monomer Conversions. <i>Macromolecules</i> , 2018, 51, 9442-9461.	2.2	14
53	Sensitivity Analysis of Single-Phase Isothermal Free Radical-Induced Grafting of Polyethylene. <i>Macromolecular Theory and Simulations</i> , 2018, 27, 1800036.	0.6	13
54	Access to the β -scission rate coefficient in acrylate radical polymerization by careful scanning of pulse laser frequencies at elevated temperature. <i>Reaction Chemistry and Engineering</i> , 2018, 3, 807-815.	1.9	25

#	ARTICLE	IF	CITATIONS
55	An evaluation of the impact of SG1 disproportionation and the addition of styrene in NMP of methyl methacrylate. <i>AIChE Journal</i> , 2018, 64, 2545-2559.	1.8	15
56	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. <i>Macromolecular Rapid Communications</i> , 2018, 39, e1800193.	2.0	47
57	Kinetic Monte Carlo Modeling Extracts Information on Chain Initiation and Termination from Complete PLP-SEC Traces. <i>Macromolecules</i> , 2017, 50, 1371-1385.	2.2	54
58	Kinetic Monte Carlo Generation of Complete Electron Spray Ionization Mass Spectra for Acrylate Macromonomer Synthesis. <i>Macromolecules</i> , 2017, 50, 2625-2636.	2.2	45
59	Estimating the photodissociation quantum yield from PLP-SEC peak heights. <i>Polymer Chemistry</i> , 2017, 8, 3124-3128.	1.9	19
60	A detailed mechanistic study of bulk MADIX of styrene and its chain extension. <i>Polymer Chemistry</i> , 2017, 8, 6948-6963.	1.9	23
61	How penultimate monomer unit effects and initiator influence ICAR ATRP of <i>n</i> -butyl acrylate and methyl methacrylate. <i>AIChE Journal</i> , 2017, 63, 4971-4986.	1.8	35
62	Modeling the reaction event history and microstructure of individual macrospecies in postpolymerization modification. <i>AIChE Journal</i> , 2017, 63, 4944-4961.	1.8	43
63	Fusing Light-Induced Step-Growth Processes with RAFT Chemistry for Segmented Copolymer Synthesis: A Synergetic Experimental and Kinetic Modeling Study. <i>Macromolecules</i> , 2017, 50, 6451-6467.	2.2	41
64	Waterborne Electrospinning of Poly(<i>N</i> -isopropylacrylamide) by Control of Environmental Parameters. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 24100-24110.	4.0	29
65	A complete understanding of the reaction kinetics for the industrial production process of expandable polystyrene. <i>AIChE Journal</i> , 2017, 63, 2043-2059.	1.8	41
66	An Update on the Pivotal Role of Kinetic Modeling for the Mechanistic Understanding and Design of Bulk and Solution RAFT Polymerization. <i>Macromolecular Theory and Simulations</i> , 2017, 26, 1600048.	0.6	54
67	<i>Ab initio</i> based kinetic Monte Carlo analysis to unravel the propagation kinetics in vinyl acetate pulsed laser polymerization. <i>Polymer Chemistry</i> , 2017, 8, 7143-7150.	1.9	35
68	Model-Based Design To Push the Boundaries of Sequence Control. <i>Macromolecules</i> , 2016, 49, 9336-9344.	2.2	51
69	A novel method for the measurement of degenerative chain transfer coefficients: proof of concept and experimental validation. <i>Polymer Chemistry</i> , 2016, 7, 3334-3349.	1.9	8
70	An alternative method to estimate the bulk backbiting rate coefficient in acrylate radical polymerization. <i>Polymer Chemistry</i> , 2016, 7, 6521-6528.	1.9	26
71	Chain Transfer in Degenerative RAFT Polymerization Revisited: A Comparative Study of Literature Methods. <i>Macromolecular Theory and Simulations</i> , 2016, 25, 104-115.	0.6	24
72	New Insights in the Treatment of Waste Water with Graphene: Dual-Site Adsorption by Sodium Dodecylbenzenesulfonate. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 9387-9396.	1.8	20

#	ARTICLE	IF	CITATIONS
73	The strength of multi-scale modeling to unveil the complexity of radical polymerization. Progress in Polymer Science, 2016, 58, 59-89.	11.8	174
74	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
75	Exploring the Full Potential of Reversible Deactivation Radical Polymerization Using Pareto-Optimal Fronts. Polymers, 2015, 7, 655-679.	2.0	24
76	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
77	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
78	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
79	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
80	Model-based design of the polymer microstructure: bridging the gap between polymer chemistry and engineering. Polymer Chemistry, 2015, 6, 7081-7096.	1.9	94
81	Fed-Batch Control and Visualization of Monomer Sequences of Individual ICAR ATRP Gradient Copolymer Chains. Polymers, 2014, 6, 1074-1095.	2.0	64
82	Controlled synthesis of poly[(butyl methacrylate)- <i>co</i> -(butyl acrylate)] via activator regenerated by electron transfer atom transfer radical polymerization: insights and improvement. Polymer International, 2014, 63, 848-857.	1.6	27
83	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
84	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
85	ARGET ATRP of Butyl Methacrylate: Utilizing Kinetic Modeling To Understand Experimental Trends. Macromolecules, 2013, 46, 3828-3840.	2.2	90
86	Comparative Kinetic Monte Carlo study of the Sulfinyl and Dithiocarbamate Precursor Route toward Highly Regioregular MDMO-PPV. Macromolecular Theory and Simulations, 2013, 22, 246-255.	0.6	15
87	A Theoretical Exploration of the Potential of ICAR ATRP for One- and Two-Pot Synthesis of Well-Defined Diblock Copolymers. Macromolecular Reaction Engineering, 2013, 7, 311-326.	0.9	42
88	Linear Gradient Quality of ATRP Copolymers. Macromolecules, 2012, 45, 8519-8531.	2.2	139
89	Kinetic Monte Carlo Modeling of the Sulfinyl Precursor Route for Poly(<i>p</i> -phenylene vinylene) Synthesis. Macromolecules, 2011, 44, 8716-8726.	2.2	55