

# Martha A Grover

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

106 papers	1,920 citations	24 h-index	40 g-index
122 ext. papers	2,337 ext. citations	5.5 avg, IF	5.11 L-index

#	Paper	IF	Citations
106	Control of Microparticle Assembly. <i>Annual Review of Control, Robotics, and Autonomous Systems</i> , <b>2022</b> , 5,	11.8	1
105	Periodic wet milling as a solution to size-based separation of crystal products from biocatalyst for continuous reactive crystallization. <i>Chemical Engineering Research and Design</i> , <b>2022</b> , 177, 473-483	5.5	1
104	Reactor Design and Optimization of -Amino Ester Hydrolase- Catalyzed Synthesis of Cephalexin.. <i>Frontiers in Bioengineering and Biotechnology</i> , <b>2022</b> , 10, 826357	5.8	
103	Effect of ion interactions on the Raman spectrum of NO <sub>3</sub> <sup>-</sup> Toward monitoring of low-activity nuclear waste at Hanford. <i>Chemical Engineering Research and Design</i> , <b>2022</b> , 181, 173-194	5.5	0
102	Urea and Acetamide Rich Solutions Circumvent the Strand Inhibition Problem to Allow Multiple Rounds of DNA and RNA Copying. <i>ChemBioChem</i> , <b>2021</b> , 23, e202100495	3.8	
101	Spectroscopic Quantification of Target Species in a Complex Mixture Using Blind Source Separation and Partial Least-Squares Regression: A Case Study on Hanford Waste. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2021</b> , 60, 9885-9896	3.9	1
100	In Situ Imaging Combined with Deep Learning for Crystallization Process Monitoring: Application to Cephalexin Production. <i>Organic Process Research and Development</i> , <b>2021</b> , 25, 1670-1679	3.9	3
99	Reactive crystallization: a review. <i>Reaction Chemistry and Engineering</i> , <b>2021</b> , 6, 364-400	4.9	16
98	Optimal Control of Crystal Size and Shape in Batch Crystallization Using a Bivariate Population Balance Modeling. <i>IFAC-PapersOnLine</i> , <b>2021</b> , 54, 653-660	0.7	1
97	Data Science Guided Experiments Identify Conjugated Polymer Solution Concentration as a Key Parameter in Device Performance <b>2021</b> , 3, 1321-1327		3
96	Kinetic model development for -Amino ester hydrolase (AEH)-catalyzed synthesis of -Lactam antibiotics. <i>Chemical Engineering Journal</i> , <b>2021</b> , 426, 131816	14.7	2
95	Chemical control of peptide material phase transitions. <i>Chemical Science</i> , <b>2021</b> , 12, 3025-3031	9.4	2
94	Optimal feedback control of batch self-assembly processes using dynamic programming. <i>Journal of Process Control</i> , <b>2020</b> , 88, 32-42	3.9	7
93	Toward data-enabled process optimization of deformable electronic polymer-based devices. <i>Current Opinion in Chemical Engineering</i> , <b>2020</b> , 27, 72-80	5.4	3
92	Small Data Machine Learning: Classification and Prediction of Poly(ethylene terephthalate) Stabilizers Using Molecular Descriptors. <i>ACS Applied Polymer Materials</i> , <b>2020</b> , 2, 5592-5601	4.3	1
91	Towards Efficient Nonenzymatic DNA Ligation: Comparing Key Parameters for Maximizing Ligation Rates and Yields with Carbodiimide Activation*. <i>ChemBioChem</i> , <b>2020</b> , 21, 3359-3370	3.8	6
90	Model development for enzymatic reactive crystallization of -Lactam antibiotics: a reaction-diffusion-crystallization approach. <i>Reaction Chemistry and Engineering</i> , <b>2020</b> , 5, 2064-2080	4.9	6

89	Understanding the Coacervate-to-Vesicle Transition of Globular Fusion Proteins to Engineer Protein Vesicle Size and Membrane Heterogeneity. <i>Biomacromolecules</i> , <b>2019</b> , 20, 3494-3503	6.9	12
88	Analysis of Multicomponent Ionic Mixtures Using Blind Source Separation: A Processing Case Study. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2019</b> , 58, 22640-22651	3.9	4
87	Control of Self-Assembly with Dynamic Programming. <i>IFAC-PapersOnLine</i> , <b>2019</b> , 52, 1-9	0.7	4
86	Control of Nucleation Density in Conjugated Polymers via Seed Nucleation. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 37955-37965	9.5	5
85	Continuous reactive crystallization of $\beta$ -lactam antibiotics catalyzed by penicillin G acylase. Part II: Case study on ampicillin and product purity. <i>Computers and Chemical Engineering</i> , <b>2019</b> , 126, 332-341	4	13
84	Systems Analysis for Peptide Systems Chemistry. <i>Life</i> , <b>2019</b> , 9,	3	1
83	Direct Observation of Growth Rate Dispersion in the Enzymatic Reactive Crystallization of Ampicillin. <i>Processes</i> , <b>2019</b> , 7, 390	2.9	1
82	Crystallization Kinetics of Cephalexin Monohydrate in the Presence of Cephalexin Precursors. <i>Crystal Growth and Design</i> , <b>2019</b> , 19, 5065-5074	3.5	8
81	Systems Chemistry: Martha Grover. <i>ChemSystemsChem</i> , <b>2019</b> , 1, e1800002	3.1	0
80	The pH dependent mechanisms of non-enzymatic peptide bond cleavage reactions. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 22, 107-113	3.6	8
79	Continuous reactive crystallization of $\beta$ -lactam antibiotics catalyzed by penicillin G acylase. Part I: Model development. <i>Computers and Chemical Engineering</i> , <b>2019</b> , 123, 331-343	4	20
78	A Prototype of a Neural, Powered, Transtibial Prosthesis for the Cat: Benchtop Characterization. <i>Frontiers in Neuroscience</i> , <b>2018</b> , 12, 471	5.1	5
77	Solving Materials Small Data Problem with Dynamic Experimental Databases. <i>Processes</i> , <b>2018</b> , 6, 79	2.9	11
76	Kinetic model discrimination of penicillin G acylase thermal deactivation by non-isothermal continuous activity assay. <i>Chemical Engineering Science</i> , <b>2018</b> , 187, 79-86	4.4	10
75	Process-Structure-Property Relationships for Design of Polymer Organic Electronics Manufacturing. <i>Computer Aided Chemical Engineering</i> , <b>2018</b> , 2467-2472	0.6	1
74	<b>2018</b> ,		1
73	A Polymer Blend Approach for Creation of Effective Conjugated Polymer Charge Transport Pathways. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 36464-36474	9.5	9
72	Incorporation of engineering knowledge into the modeling process: a local approach. <i>International Journal of Production Research</i> , <b>2017</b> , 55, 5865-5880	7.8	2

71	Using MC plots for control of paracetamol crystallization. <i>Chemical Engineering Science</i> , <b>2017</b> , 164, 344-360	12
70	Nucleation, Growth, and Alignment of Poly(3-hexylthiophene) Nanofibers for High-Performance OFETs. <i>Accounts of Chemical Research</i> , <b>2017</b> , 50, 932-942	24.3 88
69	Design of multi-phase dynamic chemical networks. <i>Nature Chemistry</i> , <b>2017</b> , 9, 799-804	17.6 46
68	Catalytic diversity in self-propagating peptide assemblies. <i>Nature Chemistry</i> , <b>2017</b> , 9, 805-809	17.6 106
67	Group Intelligence: An Active Learning Exploration of Diversity in Evolution. <i>Journal of Chemical Education</i> , <b>2017</b> , 94, 717-721	2.4 2
66	Collision cross section predictions using 2-dimensional molecular descriptors. <i>Chemical Communications</i> , <b>2017</b> , 53, 7624-7627	5.8 31
65	Modeling of Nucleation and Growth Kinetics for Unseeded Batch Cooling Crystallization. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2017</b> , 56, 4060-4073	3.9 29
64	The construction and application of Markov state models for colloidal self-assembly process control. <i>Molecular Systems Design and Engineering</i> , <b>2017</b> , 2, 78-88	4.6 10
63	High-Throughput Image Analysis of Fibrillar Materials: A Case Study on Polymer Nanofiber Packing, Alignment, and Defects in Organic Field Effect Transistors. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2017</b> , 9, 36090-36102	9.5 18
62	Surveying the sequence diversity of model prebiotic peptides by mass spectrometry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, E7652-E7659	11.5 37
61	Kinetic Model for Two-Step Nucleation of Peptide Assembly. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 7401-7411	3.4 32
60	A comparison of open-loop and closed-loop strategies in colloidal self-assembly. <i>Journal of Process Control</i> , <b>2017</b> , 60, 141-151	3.9 14
59	Elongation of Model Prebiotic Proto-Peptides by Continuous Monomer Feeding. <i>Macromolecules</i> , <b>2017</b> , 50, 9286-9294	5.5 19
58	Expanding the informational chemistries of life: peptide/RNA networks. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , <b>2017</b> , 375,	3 8
57	Multistep Conformation Selection in Amyloid Assembly. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 17007-17010	16.4 36
56	An integrated holistic model of a complex process. <i>International Journal of Advanced Manufacturing Technology</i> , <b>2017</b> , 89, 1137-1147	3.2 1
55	Automated Analysis of Orientational Order in Images of Fibrillar Materials. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 3-14	9.6 37
54	A viscous solvent enables information transfer from gene-length nucleic acids in a model prebiotic replication cycle. <i>Nature Chemistry</i> , <b>2017</b> , 9, 318-324	17.6 53

53	Batch Sequential Minimum Energy Design with Design-Region Adaptation. <i>Journal of Quality Technology</i> , <b>2017</b> , 49, 11-26	1.4	2
52	Closed-Loop Characterization of Neuronal Activation Using Electrical Stimulation and Optical Imaging. <i>Processes</i> , <b>2017</b> , 5, 30	2.9	0
51	Targeted Stimulation Using Differences in Activation Probability across the Strength-Duration Space. <i>Processes</i> , <b>2017</b> , 5, 14	2.9	1
50	Control on a molecular scale: A perspective <b>2016</b> ,		3
49	Optimal Feedback Controlled Assembly of Perfect Crystals. <i>ACS Nano</i> , <b>2016</b> , 10, 6791-8	16.7	63
48	Kinetics of prebiotic depsipeptide formation from the ester-amide exchange reaction. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 28441-28450	3.6	20
47	Externally directing self-assembly with dynamic programming <b>2016</b> ,		2
46	Data-Driven Modeling and Dynamic Programming Applied to Batch Cooling Crystallization. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2016</b> , 55, 1361-1372	3.9	17
45	Linking Models and Experiments. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2016</b> , 55, 6891-6903	3.9	50
44	Ordering of Poly(3-hexylthiophene) in Solutions and Films: Effects of Fiber Length and Grain Boundaries on Anisotropy and Mobility. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 3905-3913	9.6	80
43	Silicon Valley meets the ivory tower: Searchable data repositories for experimental nanomaterials research. <i>Current Opinion in Solid State and Materials Science</i> , <b>2016</b> , 20, 338-343	12	10
42	Markov decision process based time-varying optimal control for colloidal self-assembly. <i>IFAC-PapersOnLine</i> , <b>2016</b> , 49, 430-435	0.7	
41	Microfluidic Crystal Engineering of EConjugated Polymers. <i>ACS Nano</i> , <b>2015</b> , 9, 8220-30	16.7	94
40	Folding and imaging of DNA nanostructures in anhydrous and hydrated deep-eutectic solvents. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 6765-9	16.4	51
39	Controlling assembly of colloidal particles into structured objects: Basic strategy and a case study. <i>Journal of Process Control</i> , <b>2015</b> , 27, 64-75	3.9	25
38	Mass-Bount plots for crystal size control. <i>Chemical Engineering Science</i> , <b>2015</b> , 137, 338-351	4.4	11
37	Optimization of two-stage cooling profile in unseeded batch crystallization. <i>IFAC-PapersOnLine</i> , <b>2015</b> , 48, 297-302	0.7	6
36	Ester-Mediated Amide Bond Formation Driven by Wet-Dry Cycles: A Possible Path to Polypeptides on the Prebiotic Earth. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 9871-5	16.4	183

35	Titelbild: Folding and Imaging of DNA Nanostructures in Anhydrous and Hydrated Deep-Eutectic Solvents (Angew. Chem. 23/2015). <i>Angewandte Chemie</i> , <b>2015</b> , 127, 6753-6753	3.6	
34	Ester-Mediated Amide Bond Formation Driven by WetDry Cycles: A Possible Path to Polypeptides on the Prebiotic Earth. <i>Angewandte Chemie</i> , <b>2015</b> , 127, 10009-10013	3.6	34
33	Layers of Experiments with Adaptive Combined Design. <i>Naval Research Logistics</i> , <b>2015</b> , 62, 127-142	1.5	6
32	Folding and Imaging of DNA Nanostructures in Anhydrous and Hydrated Deep-Eutectic Solvents. <i>Angewandte Chemie</i> , <b>2015</b> , 127, 6869-6873	3.6	11
31	A Chemical Engineering Perspective on the Origins of Life. <i>Processes</i> , <b>2015</b> , 3, 309-338	2.9	13
30	Combining ATR-FTIR and FBRM for feedback on crystal size <b>2015</b> ,		3
29	Adaptive combined space-filling and D-optimal designs. <i>International Journal of Production Research</i> , <b>2015</b> , 53, 5354-5368	7.8	3
28	Feedback Control of Multicomponent Salt Crystallization. <i>Crystal Growth and Design</i> , <b>2015</b> , 15, 305-317	3.5	10
27	Shape selection and multi-stability in helical ribbons. <i>Applied Physics Letters</i> , <b>2014</b> , 104, 211901	3.4	41
26	Model identification of a template-directed peptide network for optimization in a continuous reactor. <i>Chemical Communications</i> , <b>2014</b> , 50, 3849-51	5.8	4
25	Ester Formation and Hydrolysis during WetDry Cycles: Generation of Far-from-Equilibrium Polymers in a Model Prebiotic Reaction. <i>Macromolecules</i> , <b>2014</b> , 47, 1334-1343	5.5	65
24	Application of an Empirical FBRM Model to Estimate Crystal Size Distributions in Batch Crystallization. <i>Crystal Growth and Design</i> , <b>2014</b> , 14, 607-616	3.5	35
23	Robust multicomponent IR-to-concentration model regression. <i>Chemical Engineering Science</i> , <b>2014</b> , 116, 77-90	4.4	11
22	Optimal Design of a Colloidal Self-Assembly Process. <i>IEEE Transactions on Control Systems Technology</i> , <b>2014</b> , 22, 1956-1963	4.8	14
21	Error estimation properties of Gaussian process models in stochastic simulations. <i>European Journal of Operational Research</i> , <b>2013</b> , 228, 131-140	5.6	4
20	Development of an empirical method relating crystal size distributions and FBRM measurements. <i>Chemical Engineering Science</i> , <b>2013</b> , 89, 142-151	4.4	32
19	State reduction in molecular simulations. <i>Computers and Chemical Engineering</i> , <b>2013</b> , 51, 102-110	4	10
18	Initial Experimental Design Methodology Incorporating Expert Conjecture, Prior Data, and Engineering Models for Deposition of Iridium Nanoparticles in Supercritical Carbon Dioxide. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2013</b> , 52, 9645-9653	3.9	10

17	A necessary condition for coexistence of autocatalytic replicators in a prebiotic environment. <i>Life</i> , <b>2013</b> , 3, 403-20	3	2
16	Colloidal self-assembly with Model Predictive Control <b>2013</b> ,		3
15	Optimization of a Carbon Dioxide-Assisted Nanoparticle Deposition Process Using Sequential Experimental Design with Adaptive Design Space. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2012</b> , 51, 4363-4370	3.9	19
14	Synthesis of Optically Active ZnS/Carbon Nanotube Nanocomposites in Supercritical Carbon Dioxide via a Single Source Diethyldithiocarbamate Precursor. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2012</b> , 51, 11710-11716	3.9	17
13	Optimization of carbon dioxide-assisted nanoparticle deposition process with uncertain design space. <i>Computer Aided Chemical Engineering</i> , <b>2012</b> , 1191-1195	0.6	1
12	Synthesis of Cu(2)ZnSnS(4) micro- and nanoparticles via a continuous-flow supercritical carbon dioxide process. <i>ChemSusChem</i> , <b>2012</b> , 5, 1186-9	8.3	6
11	Local-feature analysis for automated coarse-graining of bulk-polymer molecular dynamics simulations. <i>Physical Review E</i> , <b>2012</b> , 86, 061802	2.4	1
10	Universal sequence replication, reversible polymerization and early functional biopolymers: a model for the initiation of prebiotic sequence evolution. <i>PLoS ONE</i> , <b>2012</b> , 7, e34166	3.7	44
9	Gel time prediction of multifunctional acrylates using a kinetics model. <i>Polymer</i> , <b>2011</b> , 52, 866-873	3.9	21
8	Multiscale Modeling of Branch Length in Butyl Acrylate Solution Polymerization: Molecular Versus Continuum Kinetics. <i>Macromolecular Theory and Simulations</i> , <b>2011</b> , 20, 645-659	1.5	12
7	Optimization of a Chemical Vapor Deposition Process Using Sequential Experimental Design. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2010</b> , 49, 5694-5701	3.9	13
6	Multiscale Modeling of Branch Length in Butyl Acrylate Solution Polymerization. <i>Macromolecular Theory and Simulations</i> , <b>2010</b> , 19, 309-322	1.5	10
5	Stochastic dynamic predictions using Gaussian process models for nanoparticle synthesis. <i>Computers and Chemical Engineering</i> , <b>2010</b> , 34, 1953-1961	4	9
4	A new approach to batch process optimization using experimental design. <i>AIChE Journal</i> , <b>2009</b> , 55, 342-353	3.5	9
3	Principal component analysis for estimating population density from chord-length density. <i>AIChE Journal</i> , <b>2009</b> , 55, 2260-2270	3.6	7
2	Observation of Polymorphic Change through Analysis of FBRM Data: Transformation of Paracetamol from Form II to Form I. <i>Crystal Growth and Design</i> , <b>2008</b> , 8, 3316-3322	3.5	44
1	A kinetic Monte Carlo study on the nucleation mechanisms of oil-soluble initiators in the miniemulsion polymerization of styrene. <i>Journal of Polymer Science Part A</i> , <b>2008</b> , 46, 6114-6128	2.5	16