Melissa A Pasquinelli

List of Publications by Year
in descending order

57	1,191	394421	395702
papers	citations	19 h-index	33 g-index

62	62	62	1637
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Microplastic and Nanoplastic Pollution: Characterization, Transport, Fate, and Remediation Strategies. Frontiers of Environmental Science and Engineering, 2022, 16, 1.	6.0	6
2	Multiscale Constitutive Modeling of the Mechanical Properties of Polypropylene Fibers from Molecular Simulation Data. Macromolecules, 2022, 55, 728-744.	4.8	5
3	Molecular Insights into the Interfacial Properties of Cellulose Surfaces with Varying Types of Ionic Liquid Epoxies. ACS Applied Polymer Materials, 2022, 4, 3734-3742.	4.4	0
4	Xâ€ray photoelectron spectroscopy study on the photodegradation of copolyester model compounds. Journal of Applied Polymer Science, 2021, 138, 49661.	2.6	2
5	Solution size variation of linear and dendritic bis-MPA analogs using DOSY-¹H NMR. Polymer Chemistry, 2021, 12, 1507-1517.	3.9	2
6	Ammonia Sensing Performance of Polyaniline-Coated Polyamide 6 Nanofibers. ACS Omega, 2021, 6, 8950-8957.	3.5	29
7	Processâ€“Property Relationships for Melt-Spun Poly(lactic acid) Yarn. ACS Omega, 2021, 6, 15920-15928.	3.5	16
8	Effects of Ionic Liquid Nanoconfinement on the CO₂/CH₄ Separation in Poly(vinylidene fluoride)/1-Ethyl-3-methylimidazolium Thiocyanate Membranes. ACS Applied Materials & Interfaces, 2021, 13, 44460-44469.	8.0	9
9	Exploring secondary interactions and the role of temperature in moisture-contaminated polymer networks through molecular simulations. Soft Matter, 2021, 17, 2942-2956.	2.7	8
10	Hydrolytic Degradation of Polylactic Acid Fibers as a Function of pH and Exposure Time. Molecules, 2021, 26, 7554.	3.8	25
11	Bioresorbable Polymers for Surgical Suture Applications. , 2020, , 698-714.		2
12	Physical Characterization of Inclusion Complexes of Triphenyl Phosphate and Cyclodextrins in Solution. Journal of Physical Chemistry B, 2020, 124, 404-412.	2.6	4
13	Network topology and stability of homologous multiblock copolymer physical gels. Journal of Chemical Physics, 2020, 153, 124904.	3.0	5
14	Synthesis and Characterization of a Leucine-Based Block Co-Polypeptide: The Effect of the Leucine Zipper on Self-Assembly. Biomacromolecules, 2020, 21, 2463-2472.	5.4	6
15	Interfacial characteristics of a carbon nanotube-polyimide nanocomposite by molecular dynamics simulation. Nanotechnology Reviews, 2020, 9, 136-145.	5.8	43
16	Influence of UV stabilizers on the weathering of PETG and PCTT films. Journal of Applied Polymer Science, 2019, 136, 48198.	2.6	8
17	Improved Eco-Friendliness of a Common Flame Retardant through Inclusion Complexation with Cyclodextrins. ACS Applied Polymer Materials, 2019, 1, 2768-2777.	4.4	8
18	Role of Local Polymer Conformations on the Diverging Glass Transition Temperatures and Dynamic Fragilities of Isotactic-, Syndiotactic-, and Atactic-Poly(methyl methacrylate)s. Macromolecules, 2019, 52, 3897-3908.	4.8	13

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19	Photodegradation of copolyester films: A mechanistic study. Journal of Applied Polymer Science, 2019, 136, 47148.	2.6	9
20	Thermoplastic Elastomer Systems Containing Carbon Nanofibers as Soft Piezoresistive Sensors. ACS Omega, 2018, 3, 12648-12657.	3.5	22
21	Communication: Molecular-level description of constrained chain topologies in multiblock copolymer gel networks. Journal of Chemical Physics, 2018, 148, 231101.	3.0	10
22	Microphase-Separated Morphologies and Molecular Network Topologies in Multiblock Copolymer Gels. Macromolecules, 2018, 51, 5173-5181.	4.8	22
23	Nanoscale considerations responsible for diverse macroscopic phase behavior in monosubstituted isobutyl-POSS/poly(ethylene oxide) blends. Soft Matter, 2017, 13, 8672-8677.	2.7	6
24	Complex Phase Behavior and Network Characteristics of Midblock-Solvated Triblock Copolymers as Physically Cross-Linked Soft Materials. ACS Applied Materials & Interfaces, 2017, 9, 39940-39944.	8.0	15
25	Influence of Copolyester Composition on Adhesion to Soda-Lime Glass via Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2016, 8, 13583-13589.	8.0	11
26	Synthetic Design of Polyester Electrolytes Guided by Hydrophobicity Calculations. Macromolecules, 2016, 49, 7868-7876.	4.8	32
27	Physical Microfabrication of Shapeâ€Memory Polymer Systems via Bicomponent Fiber Spinning. Macromolecular Rapid Communications, 2016, 37, 1837-1843.	3.9	19
28	Hierarchical multi-component nanofiber separators for lithium polysulfide capture in lithiumâ€“sulfur batteries: an experimental and molecular modeling study. Journal of Materials Chemistry A, 2016, 4, 13572-13581.	10.3	66
29	Molecular Dynamics Simulations of Nano-biomaterials. , 2016, , 2260-2269.		0
30	Formation and characterization of an inclusion complex of triphenyl phosphate and Î²-cyclodextrin and its use as a flame retardant for polyethylene terephthalate. Polymer Degradation and Stability, 2015, 120, 244-250.	5.8	29
31	Systematic Insights from Medicinal Chemistry To Discern the Nature of Polymer Hydrophobicity. Macromolecules, 2015, 48, 7230-7236.	4.8	61
32	Communication: Molecular-level insights into asymmetric triblock copolymers: Network and phase development. Journal of Chemical Physics, 2014, 141, 121103.	3.0	27
33	Conjugated Polymer Assemblies on Carbon Nanotubes. Macromolecules, 2014, 47, 705-712.	4.8	56
34	Molecular Dynamics Simulations of the Adhesion of a Thin Annealed Film of Oleic Acid onto Crystalline Cellulose. Biomacromolecules, 2014, 15, 1476-1483.	5.4	34
35	Molecular dynamics simulations of the effect of the volume fraction on unidirectional polyimideâ€“carbon nanotube nanocomposites. Carbon, 2014, 67, 440-448.	10.3	49
36	Dissipative particle dynamics of triblock copolymer melts: A midblock conformational study at moderate segregation. Journal of Chemical Physics, 2014, 141, 244911.	3.0	33

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37	Molecular Dynamics Simulations for Predicting Surface Wetting. AIMS Materials Science, 2014, 1, 121-131.	1.4	12
38	Mesoscopic Simulations of the Phase Behavior of Aqueous EO₁₉PO₂₉EO₁₉ Solutions Confined and Sheared by Hydrophobic and Hydrophilic Surfaces. ACS Applied Materials & Interfaces, 2012, 4, 87-95.	8.0	17
39	Experimental and Computational Study of the Effect of Alcohols on the Solution and Adsorption Properties of a Nonionic Symmetric Triblock Copolymer. Journal of Physical Chemistry B, 2012, 116, 1289-1298.	2.6	10
40	Molecular Dynamics Simulations of the Thermal Stability of Crystalline Cellulose Surfaces Coated with Oleic Acid. ACS Symposium Series, 2012, , 191-208.	0.5	1
41	Molecular Dynamics Simulations of Interactions between Polyanilines in Their Inclusion Complexes with Î²-Cyclodextrins. Journal of Physical Chemistry B, 2012, 116, 2023-2030.	2.6	17
42	The Soft-Confined Method for Creating Molecular Models of Amorphous Polymer Surfaces. Journal of Physical Chemistry B, 2012, 116, 1570-1578.	2.6	30
43	In Silico Strategies for Modeling Stereoselective Metabolism of Pyrethroids. ACS Symposium Series, 2012, , 245-269.	0.5	2
44	Unexpected Results from the Comparison of Solid-State Conformations and ¹³C NMR Spectra of Poly (trimethylene terephthalate) and Its Model Compounds. Macromolecules, 2011, 44, 7050-7055.	4.8	3
45	Adapting Visualâ€Analytical Tools for the Exploration of Structural and Dynamical Features of Polymer Conformations. Macromolecular Theory and Simulations, 2011, 20, 286-298.	1.4	3
46	Exploration of polymer conformational similarities in polymer-carbon nanotube interfaces. , 2010, , .		0
47	Molecular Dynamics Simulations of Flexible Polymer Chains Wrapping Single-Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2010, 114, 4122-4129.	2.6	184
48	Molecular Dynamics Simulations of Polymers with Stiff Backbones Interacting with Single-Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2010, 114, 9349-9355.	2.6	114
49	Visualization of the Molecular Dynamics of Polymers and Carbon Nanotubes. Lecture Notes in Computer Science, 2009, , 129-139.	1.3	1
50	Computational Molecular Modeling for Evaluating the Toxicity of Environmental Chemicals: Prioritizing Bioassay Requirements. Environmental Health Perspectives, 2008, 116, 573-577.	6.0	41
51	Protein Phosphorylation and Intermolecular Electron Transfer:Â A Joint Experimental and Computational Study of a Hormone Biosynthesis Pathway. Journal of the American Chemical Society, 2007, 129, 4206-4216.	13.7	21
52	Binding of Warfarin Influences the Acid-Base Equilibrium of H242 in Sudlow Site I of Human Serum Albumin. Photochemistry and Photobiology, 2006, 82, 1365.	2.5	27
53	Quantum chemical investigation of biexcitons in conjugated polymers. Journal of Chemical Physics, 2003, 118, 8082-8092.	3.0	11
54	Energy landscapes for effective particles in conjugated polymers. Synthetic Metals, 1999, 101, 518-519.	3.9	1

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55	Cyclization kinetics of gelâ€spun polyacrylonitrile/aldaricâ€acid sugars using the isoconversional approach. Journal of Applied Polymer Science, 0, , 51789.	2.6	1
56	Combined experimental and computational study of process-property relationships for bioabsorbable polymers. Frontiers in Bioengineering and Biotechnology, 0, 4, .	4.1	0
57	Integrating Computing into Thermodynamics: Lessons Learned. , 0, , .		0