

# Melissa A Pasquinelli

## List of Publications by Year in descending order

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57  
papers

1,191  
citations

394421

19  
h-index

395702

33  
g-index

62  
all docs

62  
docs citations

62  
times ranked

1637  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Dynamics Simulations of Flexible Polymer Chains Wrapping Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 4122-4129.	2.6	184
2	Molecular Dynamics Simulations of Polymers with Stiff Backbones Interacting with Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2010, 114, 9349-9355.	2.6	114
3	Hierarchical multi-component nanofiber separators for lithium polysulfide capture in lithium-sulfur batteries: an experimental and molecular modeling study. <i>Journal of Materials Chemistry A</i> , 2016, 4, 13572-13581.	10.3	66
4	Systematic Insights from Medicinal Chemistry To Discern the Nature of Polymer Hydrophobicity. <i>Macromolecules</i> , 2015, 48, 7230-7236.	4.8	61
5	Conjugated Polymer Assemblies on Carbon Nanotubes. <i>Macromolecules</i> , 2014, 47, 705-712.	4.8	56
6	Molecular dynamics simulations of the effect of the volume fraction on unidirectional polyimide-carbon nanotube nanocomposites. <i>Carbon</i> , 2014, 67, 440-448.	10.3	49
7	Interfacial characteristics of a carbon nanotube-polyimide nanocomposite by molecular dynamics simulation. <i>Nanotechnology Reviews</i> , 2020, 9, 136-145.	5.8	43
8	Computational Molecular Modeling for Evaluating the Toxicity of Environmental Chemicals: Prioritizing Bioassay Requirements. <i>Environmental Health Perspectives</i> , 2008, 116, 573-577.	6.0	41
9	Molecular Dynamics Simulations of the Adhesion of a Thin Annealed Film of Oleic Acid onto Crystalline Cellulose. <i>Biomacromolecules</i> , 2014, 15, 1476-1483.	5.4	34
10	Dissipative particle dynamics of triblock copolymer melts: A midblock conformational study at moderate segregation. <i>Journal of Chemical Physics</i> , 2014, 141, 244911.	3.0	33
11	Synthetic Design of Polyester Electrolytes Guided by Hydrophobicity Calculations. <i>Macromolecules</i> , 2016, 49, 7868-7876.	4.8	32
12	The Soft-Confined Method for Creating Molecular Models of Amorphous Polymer Surfaces. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1570-1578.	2.6	30
13	Formation and characterization of an inclusion complex of triphenyl phosphate and $\beta$ -cyclodextrin and its use as a flame retardant for polyethylene terephthalate. <i>Polymer Degradation and Stability</i> , 2015, 120, 244-250.	5.8	29
14	Ammonia Sensing Performance of Polyaniline-Coated Polyamide 6 Nanofibers. <i>ACS Omega</i> , 2021, 6, 8950-8957.	3.5	29
15	Binding of Warfarin Influences the Acid-Base Equilibrium of H242 in Sudlow Site I of Human Serum Albumin. <i>Photochemistry and Photobiology</i> , 2006, 82, 1365.	2.5	27
16	Communication: Molecular-level insights into asymmetric triblock copolymers: Network and phase development. <i>Journal of Chemical Physics</i> , 2014, 141, 121103.	3.0	27
17	Hydrolytic Degradation of Polylactic Acid Fibers as a Function of pH and Exposure Time. <i>Molecules</i> , 2021, 26, 7554.	3.8	25
18	Thermoplastic Elastomer Systems Containing Carbon Nanofibers as Soft Piezoresistive Sensors. <i>ACS Omega</i> , 2018, 3, 12648-12657.	3.5	22

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19	Microphase-Separated Morphologies and Molecular Network Topologies in Multiblock Copolymer Gels. <i>Macromolecules</i> , 2018, 51, 5173-5181.	4.8	22
20	Protein Phosphorylation and Intermolecular Electron Transfer: A Joint Experimental and Computational Study of a Hormone Biosynthesis Pathway. <i>Journal of the American Chemical Society</i> , 2007, 129, 4206-4216.	13.7	21
21	Physical Microfabrication of Shape-Memory Polymer Systems via Bicomponent Fiber Spinning. <i>Macromolecular Rapid Communications</i> , 2016, 37, 1837-1843.	3.9	19
22	Mesoscopic Simulations of the Phase Behavior of Aqueous EO <sub>19</sub> PO <sub>29</sub> EO <sub>19</sub> Solutions Confined and Sheared by Hydrophobic and Hydrophilic Surfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2012, 4, 87-95.	8.0	17
23	Molecular Dynamics Simulations of Interactions between Polyanilines in Their Inclusion Complexes with $\beta$ -Cyclodextrins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2023-2030.	2.6	17
24	Process-Property Relationships for Melt-Spun Poly(lactic acid) Yarn. <i>ACS Omega</i> , 2021, 6, 15920-15928.	3.5	16
25	Complex Phase Behavior and Network Characteristics of Midblock-Solvated Triblock Copolymers as Physically Cross-Linked Soft Materials. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 39940-39944.	8.0	15
26	Role of Local Polymer Conformations on the Diverging Glass Transition Temperatures and Dynamic Fragilities of Isotactic-, Syndiotactic-, and Atactic-Poly(methyl methacrylate)s. <i>Macromolecules</i> , 2019, 52, 3897-3908.	4.8	13
27	Molecular Dynamics Simulations for Predicting Surface Wetting. <i>AIMS Materials Science</i> , 2014, 1, 121-131.	1.4	12
28	Quantum chemical investigation of biexcitons in conjugated polymers. <i>Journal of Chemical Physics</i> , 2003, 118, 8082-8092.	3.0	11
29	Influence of Copolyester Composition on Adhesion to Soda-Lime Glass via Molecular Dynamics Simulations. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 13583-13589.	8.0	11
30	Experimental and Computational Study of the Effect of Alcohols on the Solution and Adsorption Properties of a Nonionic Symmetric Triblock Copolymer. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1289-1298.	2.6	10
31	Communication: Molecular-level description of constrained chain topologies in multiblock copolymer gel networks. <i>Journal of Chemical Physics</i> , 2018, 148, 231101.	3.0	10
32	Photodegradation of copolyester films: A mechanistic study. <i>Journal of Applied Polymer Science</i> , 2019, 136, 47148.	2.6	9
33	Effects of Ionic Liquid Nanoconfinement on the CO <sub>2</sub> /CH <sub>4</sub> Separation in Poly(vinylidene fluoride)/1-Ethyl-3-methylimidazolium Thiocyanate Membranes. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 44460-44469.	8.0	9
34	Influence of UV stabilizers on the weathering of PETG and PCTT films. <i>Journal of Applied Polymer Science</i> , 2019, 136, 48198.	2.6	8
35	Improved Eco-Friendliness of a Common Flame Retardant through Inclusion Complexation with Cyclodextrins. <i>ACS Applied Polymer Materials</i> , 2019, 1, 2768-2777.	4.4	8
36	Exploring secondary interactions and the role of temperature in moisture-contaminated polymer networks through molecular simulations. <i>Soft Matter</i> , 2021, 17, 2942-2956.	2.7	8

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37	Nanoscale considerations responsible for diverse macroscopic phase behavior in monosubstituted isobutyl-POSS/poly(ethylene oxide) blends. <i>Soft Matter</i> , 2017, 13, 8672-8677.	2.7	6
38	Synthesis and Characterization of a Leucine-Based Block Co-Polypeptide: The Effect of the Leucine Zipper on Self-Assembly. <i>Biomacromolecules</i> , 2020, 21, 2463-2472.	5.4	6
39	Microplastic and Nanoplastic Pollution: Characterization, Transport, Fate, and Remediation Strategies. <i>Frontiers of Environmental Science and Engineering</i> , 2022, 16, 1.	6.0	6
40	Network topology and stability of homologous multiblock copolymer physical gels. <i>Journal of Chemical Physics</i> , 2020, 153, 124904.	3.0	5
41	Multiscale Constitutive Modeling of the Mechanical Properties of Polypropylene Fibers from Molecular Simulation Data. <i>Macromolecules</i> , 2022, 55, 728-744.	4.8	5
42	Physical Characterization of Inclusion Complexes of Triphenyl Phosphate and Cyclodextrins in Solution. <i>Journal of Physical Chemistry B</i> , 2020, 124, 404-412.	2.6	4
43	Unexpected Results from the Comparison of Solid-State Conformations and <sup>13</sup> C NMR Spectra of Poly(trimethylene terephthalate) and Its Model Compounds. <i>Macromolecules</i> , 2011, 44, 7050-7055.	4.8	3
44	Adapting Visual Analytical Tools for the Exploration of Structural and Dynamical Features of Polymer Conformations. <i>Macromolecular Theory and Simulations</i> , 2011, 20, 286-298.	1.4	3
45	In Silico Strategies for Modeling Stereoselective Metabolism of Pyrethroids. <i>ACS Symposium Series</i> , 2012, , 245-269.	0.5	2
46	Bioresorbable Polymers for Surgical Suture Applications. , 2020, , 698-714.		2
47	X-ray photoelectron spectroscopy study on the photodegradation of copolyester model compounds. <i>Journal of Applied Polymer Science</i> , 2021, 138, 49661.	2.6	2
48	Solution size variation of linear and dendritic bis-MPA analogs using DOSY- <sup>1</sup> H NMR. <i>Polymer Chemistry</i> , 2021, 12, 1507-1517.	3.9	2
49	Energy landscapes for effective particles in conjugated polymers. <i>Synthetic Metals</i> , 1999, 101, 518-519.	3.9	1
50	Visualization of the Molecular Dynamics of Polymers and Carbon Nanotubes. <i>Lecture Notes in Computer Science</i> , 2009, , 129-139.	1.3	1
51	Molecular Dynamics Simulations of the Thermal Stability of Crystalline Cellulose Surfaces Coated with Oleic Acid. <i>ACS Symposium Series</i> , 2012, , 191-208.	0.5	1
52	Cyclization kinetics of gel-spun polyacrylonitrile/aldaric acid sugars using the isoconversional approach. <i>Journal of Applied Polymer Science</i> , 0, , 51789.	2.6	1
53	Exploration of polymer conformational similarities in polymer-carbon nanotube interfaces. , 2010, ,		0
54	Combined experimental and computational study of process-property relationships for bioabsorbable polymers. <i>Frontiers in Bioengineering and Biotechnology</i> , 0, 4, .	4.1	0

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55	Molecular Dynamics Simulations of Nano-biomaterials. , 2016, , 2260-2269.		0
56	Integrating Computing into Thermodynamics: Lessons Learned. , 0, , .		0
57	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