Arthi Jayaraman

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4930981/publications.pdf

Version: 2024-02-01

110 papers	3,422 citations	147566 31 h-index	168136 53 g-index
111 all docs	111 docs citations	111 times ranked	3199 citing authors

#	Article	IF	Citations
1	Modeling and Simulations of Polymers: A Roadmap. Macromolecules, 2019, 52, 755-786.	2.2	298
2	Theory and simulation studies of effective interactions, phase behavior and morphology in polymer nanocomposites. Soft Matter, 2014, 10, 13-38.	1.2	231
3	Unraveling the Structure and Function of Melanin through Synthesis. Journal of the American Chemical Society, 2021, 143, 2622-2637.	6.6	174
4	Molecular theories of polymer nanocomposites. Current Opinion in Solid State and Materials Science, 2010, 14, 38-48.	5.6	150
5	Effective Interactions and Self-Assembly of Hybrid Polymer Grafted Nanoparticles in a Homopolymer Matrix. Macromolecules, 2009, 42, 8423-8434.	2.2	104
6	Polydispersity for Tuning the Potential of Mean Force between Polymer Grafted Nanoparticles in a Polymer Matrix. Physical Review Letters, 2013, 110, 018301.	2.9	85
7	Effective Interactions, Structure, and Phase Behavior of Lightly Tethered Nanoparticles in Polymer Melts. Macromolecules, 2008, 41, 9430-9438.	2.2	84
8	Understanding the Effect of Polylysine Architecture on DNA Binding Using Molecular Dynamics Simulations. Biomacromolecules, 2011, 12, 3870-3879.	2.6	78
9	Polymer grafted nanoparticles: Effect of chemical and physical heterogeneity in polymer grafts on particle assembly and dispersion. Journal of Polymer Science, Part B: Polymer Physics, 2013, 51, 524-534.	2.4	73
10	Wettingâ€“Dewetting and Dispersionâ€“Aggregation Transitions Are Distinct for Polymer Grafted Nanoparticles in Chemically Dissimilar Polymer Matrix. Journal of the American Chemical Society, 2015, 137, 10624-10631.	6.6	73
11	Structure and assembly of dense solutions and melts of single tethered nanoparticles. Journal of Chemical Physics, 2008, 128, 164904.	1.2	69
12	Computationally Linking Molecular Features of Conjugated Polymers and Fullerene Derivatives to Bulk Heterojunction Morphology. Macromolecules, 2013, 46, 5775-5785.	2.2	64
13	Effect of the Number and Placement of Polymer Tethers on the Structure of Concentrated Solutions and Melts of Hybrid Nanoparticles. Langmuir, 2008, 24, 11119-11130.	1.6	62
14	Self-Consistent PRISM Theoryâ^'Monte Carlo Simulation Studies of Copolymer Grafted Nanoparticles in a Homopolymer Matrix. Macromolecules, 2010, 43, 8251-8263.	2.2	56
15	Molecular Dynamics Simulation and PRISM Theory Study of Assembly in Solutions of Amphiphilic Bottlebrush Block Copolymers. Macromolecules, 2018, 51, 7586-7599.	2.2	54
16	Identifying the Ideal Characteristics of the Grafted Polymer Chain Length Distribution for Maximizing Dispersion of Polymer Grafted Nanoparticles in a Polymer Matrix. Macromolecules, 2013, 46, 9144-9150.	2.2	50
17	Effect of bidispersity in grafted chain length on grafted chain conformations and potential of mean force between polymer grafted nanoparticles in a homopolymer matrix. Journal of Chemical Physics, 2011, 134, 194906.	1.2	49
18	Effect of Peptide Sequence on the LCST-Like Transition of Elastin-Like Peptides and Elastin-Like Peptideâ€“Collagen-Like Peptide Conjugates: Simulations and Experiments. Biomacromolecules, 2019, 20, 1178-1189.	2.6	48

#	Article	IF	Citations
19	Molecular dynamics simulation study of linear, bottlebrush, and star-like amphiphilic block polymer assembly in solution. Soft Matter, 2019, 15, 3987-3998.	1.2	46
20	Polydisperse homopolymer grafts stabilize dispersions of nanoparticles in a chemically identical homopolymer matrix: an integrated theory and simulation study. Soft Matter, 2013, 9, 6876.	1.2	43
21	pyPRISM: A Computational Tool for Liquid-State Theory Calculations of Macromolecular Materials. Macromolecules, 2018, 51, 2906-2922.	2.2	43
22	The Good Host: Formation of Discrete One-Dimensional Fullerene â€œChannelsâ€•in Well-Ordered Poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-‹i›b‹/i›]thiophene) Oligomers. Journal of the American Chemical Society, 2014, 136, 18120-18130.	6.6	42
23	Diblock Copolymer Grafted Particles as Compatibilizers for Immiscible Binary Homopolymer Blends. ACS Macro Letters, 2015, 4, 155-159.	2.3	41
24	Monte carlo simulations of polydisperse polymers grafted on spherical surfaces. Journal of Polymer Science, Part B: Polymer Physics, 2012, 50, 694-705.	2.4	39
25	Assembly of copolymer functionalized nanoparticles: a Monte Carlo simulation study. Soft Matter, 2011, 7, 5952.	1.2	37
26	Effect of conjugation on phase transitions in thermoresponsive polymers: an atomistic and coarse-grained simulation study. Soft Matter, 2017, 13, 2907-2918.	1.2	37
27	Effect of Polymer Architecture on the Structure and Interactions of Polymer Grafted Particles: Theory and Simulations. Macromolecules, 2017, 50, 4854-4866.	2.2	37
28	100th Anniversary of Macromolecular Science Viewpoint: Modeling and Simulation of Macromolecules with Hydrogen Bonds: Challenges, Successes, and Opportunities. ACS Macro Letters, 2020, 9, 656-665.	2.3	37
29	Integrating PRISM theory and Monte Carlo simulation to study polymer-functionalised particles and polymer nanocomposites. Molecular Simulation, 2012, 38, 751-761.	0.9	36
30	Effect of backbone chemistry on hybridization thermodynamics of oligonucleic acids: a coarse-grained molecular dynamics simulation study. Soft Matter, 2016, 12, 2276-2287.	1.2	36
31	Scaling Exponent and Effective Interactions in Linear and Cyclic Polymer Solutions: Theory, Simulations, and Experiments. Macromolecules, 2019, 52, 4579-4589.	2.2	35
32	Controlling the Morphology of Model Conjugated Thiophene Oligomers through Alkyl Side Chain Length, Placement, and Interactions. Macromolecules, 2014, 47, 2736-2747.	2.2	34
33	Interaction of Hyaluronan Binding Peptides with Glycosaminoglycans in Poly(ethylene glycol) Hydrogels. Biomacromolecules, 2014, 15, 1132-1141.	2.6	34
34	Decreasing Polymer Flexibility Improves Wetting and Dispersion of Polymer-Grafted Particles in a Chemically Identical Polymer Matrix. ACS Macro Letters, 2014, 3, 628-632.	2.3	33
35	Using Theory and Simulations To Calculate Effective Interactions in Polymer Nanocomposites with Polymer-Grafted Nanoparticles. Macromolecules, 2016, 49, 9684-9692.	2.2	31
36	Computer Simulation Study of Molecular Recognition in Model DNA Microarrays. Biophysical Journal, 2006, 91, 2227-2236.	0.2	30

#	Article	IF	Citations
37	Hybrid Atomistic and Coarse-Grained Molecular Dynamics Simulations of Polyethylene Glycol (PEG) in Explicit Water. Journal of Physical Chemistry B, 2016, 120, 4160-4173.	1.2	29
38	Development of a Coarse-Grained Model of Collagen-Like Peptide (CLP) for Studies of CLP Triple Helix Melting. Journal of Physical Chemistry B, 2018, 122, 1929-1939.	1.2	29
39	Impact of Hydrogen Bonding Interactions on Graftâ€“Matrix Wetting and Structure in Polymer Nanocomposites. Macromolecules, 2019, 52, 2725-2735.	2.2	29
40	Liquid state theory of the structure and phase behaviour of polymer-tethered nanoparticles in dense suspensions, melts and nanocomposites. Molecular Simulation, 2009, 35, 835-848.	0.9	28
41	Effect of Hydrophobic and Hydrophilic Surfaces on the Stability of Double-Stranded DNA. Biomacromolecules, 2015, 16, 1862-1869.	2.6	28
42	Molecular Modeling and Simulations of Peptideâ€“Polymer Conjugates. Annual Review of Chemical and Biomolecular Engineering, 2020, 11, 257-276.	3.3	28
43	Assembly of Amphiphilic Block Copolymers and Nanoparticles in Solution: Coarse-Grained Molecular Simulation Study. Journal of Chemical & Engineering Data, 2018, 63, 2351-2367.	1.0	27
44	Structure and thermodynamics of ssDNA oligomers near hydrophobic and hydrophilic surfaces. Soft Matter, 2013, 9, 11521.	1.2	26
45	PRISM Theory Study of Amphiphilic Block Copolymer Solutions with Varying Copolymer Sequence and Composition. Macromolecules, 2017, 50, 7419-7431.	2.2	25
46	Computational Reverse-Engineering Analysis for Scattering Experiments on Amphiphilic Block Polymer Solutions. Journal of the American Chemical Society, 2019, 141, 14916-14930.	6.6	24
47	Experiments and Simulations of Complex Sugar-Based Coilâ^'Brush Block Polymer Nanoassemblies in Aqueous Solution. ACS Nano, 2019, 13, 5147-5162.	7.3	23
48	Effect of monomer sequences on conformations of copolymers grafted on spherical nanoparticles: A Monte Carlo simulation study. Journal of Chemical Physics, 2010, 132, 164901.	1.2	22
49	Effect of matrix bidispersity on the morphology of polymerâ€grafted nanoparticleâ€filled polymer nanocomposites. Journal of Polymer Science, Part B: Polymer Physics, 2014, 52, 1661-1668.	2.4	21
50	Molecular Modeling and Simulation of Polymer Nanocomposites with Nanorod Fillers. Journal of Physical Chemistry B, 2021, 125, 2435-2449.	1.2	21
51	Coarse-Grained Simulation Studies of Effects of Polycation Architecture on Structure of the Polycation and Polycationâ€“Polyanion Complexes. Macromolecules, 2012, 45, 8083-8096.	2.2	20
52	Molecular simulation study of the assembly of DNA-functionalised nanoparticles: Effect of DNA strand sequence and composition. Molecular Simulation, 2013, 39, 741-753.	0.9	20
53	Tuning the wettingâ€“dewetting and dispersionâ€“aggregation transitions in polymer nanocomposites using composition of graft and matrix polymers. Materials Research Express, 2016, 3, 034001.	0.8	20
54	Placement of tyrosine residues as a design element for tuning the phase transition of elastin-peptide-containing conjugates: experiments and simulations. Molecular Systems Design and Engineering, 2020, 5, 1239-1254.	1.7	20

#	Article	IF	Citations
55	Assembly of diblock copolymer functionalized spherical nanoparticles as a function of copolymer composition. Journal of Chemical Physics, 2014, 140, 144905.	1.2	19
56	Experimental and theoretical evidence for molecular forces driving surface segregation in photonic colloidal assemblies. Science Advances, 2019, 5, eaax1254.	4.7	19
57	Dispersion and Aggregation of Polymer Grafted Particles in Polymer Nanocomposites Driven by the Hardness and Size of the Grafted Layer Tuned by Attractive Graftâ€“Matrix Interactions. Macromolecules, 2020, 53, 1302-1313.	2.2	19
58	Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) with Machine Learning Enhancement to Determine Structure of Nanoparticle Mixtures and Solutions. ACS Central Science, 2022, 8, 996-1007.	5.3	19
59	Molecular Simulations of Polycationâ€“DNA Binding Exploring the Effect of Peptide Chemistry and Sequence in Nuclear Localization Sequence Based Polycations. Journal of Physical Chemistry B, 2013, 117, 11988-11999.	1.2	18
60	Anisotropic Synthetic Allomelanin Materials via Solidâ€State Polymerization of Selfâ€Assembled 1,8â€Dihydroxynaphthalene Dimers. Angewandte Chemie - International Edition, 2021, 60, 17464-17471.	7.2	18
61	Machine Learning Enhanced Computational Reverse Engineering Analysis for Scattering Experiments (CREASE) to Determine Structures in Amphiphilic Polymer Solutions. ACS Polymers Au, 2021, 1, 153-164.	1.7	18
62	Hierarchical Self-Assembly of Poly(<scp>d</scp>-glucose carbonate) Amphiphilic Block Copolymers in Mixed Solvents. Macromolecules, 2020, 53, 8581-8591.	2.2	17
63	Effect of blockiness in grafted monomer sequences on assembly of copolymer grafted nanoparticles: a Monte Carlo simulation study. Soft Matter, 2013, 9, 155-169.	1.2	16
64	Dispersing Zwitterions into Comb Polymers for Nonviral Transfection: Experiments and Molecular Simulation. Biomacromolecules, 2016, 17, 546-557.	2.6	16
65	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
66	Effect of homopolymer matrix on diblock copolymer grafted nanoparticle conformation and potential of mean force: A molecular simulation study. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 76-88.	2.4	15
67	Effects of Polymer Conjugation on Hybridization Thermodynamics of Oligonucleic Acids. Journal of Physical Chemistry B, 2016, 120, 9788-9799.	1.2	15
68	Self-assembly of amphiphilic polymers of varying architectures near attractive surfaces. Soft Matter, 2020, 16, 623-633.	1.2	15
69	Computational Reverse-Engineering Analysis of Scattering Experiments (CREASE) on Amphiphilic Block Polymer Solutions: Cylindrical and Fibrillar Assembly. Macromolecules, 2021, 54, 783-796.	2.2	15
70	Structural Color Production in Melaninâ€Based Disordered Colloidal Nanoparticle Assemblies in Spherical Confinement. Advanced Optical Materials, 2022, 10, .	3.6	15
71	Computational Design of Oligopeptide Containing Poly(ethylene glycol) Brushes for Stimuli-Responsive Drug Delivery. Journal of Physical Chemistry B, 2015, 119, 13309-13320.	1.2	14
72	Development of a New Coarse-Grained Model to Simulate Assembly of Cellulose Chains Due to Hydrogen Bonding. Journal of Chemical Theory and Computation, 2020, 16, 4599-4614.	2.3	14

#	Article	IF	Citations
73	Interfacial Compatibilization in Ternary Polymer Nanocomposites: Comparing Theory and Experiments. Macromolecules, 2021, 54, 797-811.	2.2	14
74	Coarse-grained molecular dynamics simulations of Î±-1,3-glucan. Soft Matter, 2019, 15, 4669-4681.	1.2	13
75	Self-Assembly of Allomelanin Dimers and the Impact of Poly(ethylene glycol) on the Assembly: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2020, 124, 2702-2714.	1.2	13
76	Sequence-Specific Recognition of Cancer Drug-DNA Adducts by HMGB1a Repair Protein. Biophysical Journal, 2012, 102, 2331-2338.	0.2	11
77	Effect of oligonucleic acid (ONA) backbone features on assembly of ONAâ€“star polymer conjugates: a coarse-grained molecular simulation study. Soft Matter, 2017, 13, 6770-6783.	1.2	11
78	Impact of Composition and Placement of Hydrogen-Bonding Groups along Polymer Chains on Blend Phase Behavior: Coarse-Grained Molecular Dynamics Simulation Study. Macromolecules, 2022, 55, 2675-2690.	2.2	11
79	Macromolecular â€˜sizeâ€™ and â€˜hardnessâ€™ drives structure in solvent-swollen blends of linear, cyclic, and star polymers. Soft Matter, 2018, 14, 411-423.	1.2	10
80	Combining simulations and experiments for the molecular engineering of multifunctional collagen mimetic peptide-based materials. Soft Matter, 2021, 17, 1985-1998.	1.2	10
81	Morphological studies of blends of conjugated polymers and acceptor molecules using langevin dynamics simulations. Journal of Polymer Science, Part B: Polymer Physics, 2013, 51, 64-77.	2.4	9
82	Molecular simulation study of assembly of DNA-grafted nanoparticles: effect of bidispersity in DNA strand length. Molecular Simulation, 2014, 40, 1085-1098.	0.9	9
83	Surface composition and ordering of binary nanoparticle mixtures in spherical confinement. Molecular Systems Design and Engineering, 2020, 5, 864-875.	1.7	9
84	Computational Reverse-Engineering Analysis for Scattering Experiments of Assembled Binary Mixture of Nanoparticles. ACS Materials Au, 2021, 1, 140-156.	2.6	9
85	Effect of Nanorod Physical Roughness on the Aggregation and Percolation of Nanorods in Polymer Nanocomposites. ACS Macro Letters, 2021, 10, 1416-1422.	2.3	9
86	Simulation study of the effects of surface chemistry and temperature on the conformations of ssDNA oligomers near hydrophilic and hydrophobic surfaces. Journal of Chemical Physics, 2014, 140, .	1.2	8
87	Molecular dynamics simulations and PRISM theory study of solutions of nanoparticles and triblock copolymers with solvophobic end blocks. Molecular Systems Design and Engineering, 2018, 3, 453-472.	1.7	8
88	Melting thermodynamics of oligonucleic acids conjugated with relatively solvophobic linear polymers: A coarseâ€grained molecular simulation study. Journal of Polymer Science, Part B: Polymer Physics, 2019, 57, 1196-1208.	2.4	8
89	ssDNA-amphiphile architecture used to control dimensions of DNA nanotubes. Nanoscale, 2019, 11, 19850-19861.	2.8	8
90	Computational Reverse Engineering Analysis for Scattering Experiments (CREASE) on Vesicles Assembled from Amphiphilic Macromolecular Solutions. Jacs Au, 2021, 1, 1925-1936.	3.6	8

#	Article	IF	Citations
91	Leveraging Gibbs Ensemble Molecular Dynamics and Hybrid Monte Carlo/Molecular Dynamics for Efficient Study of Phase Equilibria. Journal of Chemical Theory and Computation, 2016, 12, 5501-5510.	2.3	7
92	Role of structure and dynamics of DNA with cisplatin and oxaliplatin adducts in various sequence contexts on binding of HMGB1a. Molecular Simulation, 2012, 38, 793-808.	0.9	5
93	Effect of additive length and chemistry on the morphology of blends of conjugated thiophenes and fullerene derivative acceptor molecules. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 1046-1057.	2.4	5
94	Development of Coarse-Grained Models for Poly(4-vinylphenol) and Poly(2-vinylpyridine): Polymer Chemistries with Hydrogen Bonding. Polymers, 2020, 12, 2764.	2.0	5
95	Impact of collagen-like peptide (CLP) heterotrimeric triple helix design on helical thermal stability and hierarchical assembly: a coarse-grained molecular dynamics simulation study. Soft Matter, 2022, 18, 3177-3192.	1.2	3
96	Effect of side chain length on the morphology of blends of 2,5â€bis(3â€alkylthiophenâ€2â€yl)thieno[3,2â€b]thiophene oligomers and fullerene derivatives. Journal of Polymer Science, Part B: Polymer Physics, 2016, 54, 89-97.	2.4	2
97	Understanding the Effect of Heterogeneous Particle Functionalization on Graftâ€“Matrix Wetting and Structure in Polymer Nanocomposites Containing Grafted Nanoparticles Using Multiscale Modeling and Simulation. ACS Applied Polymer Materials, 2021, 3, 5642-5655.	2.0	2
98	Inaugural Editorial for ACS Polymers Au. ACS Polymers Au, 0, , .	1.7	1
99	Design and Implementation of pyPRISM: A Polymer Liquid-State Theory Framework. , 2018, , .		1
100	pyPRISM: A Computational Tool for Liquid-State Theory Calculations of Macromolecular Materials. Macromolecules, 2018, 51, .	2.2	1
101	Publishing in and Reviewing for ACS Polymers Au. ACS Polymers Au, 2021, 1, 131-133.	1.7	1
102	Molecular design and engineering of biomimetic, bioinspired and biologically derived materials. Molecular Systems Design and Engineering, 2020, 5, 599-601.	1.7	0
103	Coarse-Grained Modeling and Simulations of Thermoresponsive Biopolymers and Polymer Nanocomposites with Specific and Directional Interactions. Molecular Modeling and Simulation, 2021, , 37-74.	0.2	0
104	Anisotropic Synthetic Allomelanin Materials via Solidâ€State Polymerization of Selfâ€Assembled 1,8â€Dihydroxynaphthalene Dimers. Angewandte Chemie, 2021, 133, 17605-17612.	1.6	0
105	Titelbild: Anisotropic Synthetic Allomelanin Materials via Solidâ€State Polymerization of Selfâ€Assembled 1,8â€Dihydroxynaphthalene Dimers (Angew. Chem. 32/2021). Angewandte Chemie, 2021, 133, 17361-17361.	1.6	0
106	ACS Polymers Auâ€™s First Issue. ACS Polymers Au, 2021, 1, 1-3.	1.7	0
107	A Tribute to Carol K. Hall. Journal of Physical Chemistry B, 2021, 125, 11341-11342.	1.2	0
108	Polymer Reference Interaction Site Model (PRISM) Theory and Molecular Simulation Studies of Polymer Nanocomposites. Springer Series in Materials Science, 2021, , 1-22.	0.4	0

#	Article	IF	Citations
109	ACS Polymers Auâ€™s Most Viewed Papers in 2021. ACS Polymers Au, 2022, 2, 1-2.	1.7	0
110	ACS Polymers Au Recognizes Rising Stars in Polymers in 2021. ACS Polymers Au, 2022, 2, 3-7.	1.7	0