Gary S Grest

List of Publications by Year
in descending order

147 papers	14,442 citations	34105 52 h-index	19190 118 g-index
148 all docs	148 docs citations	148 times ranked	8234 citing authors

#	Article	IF	Citations
1	Dynamics of entangled linear polymer melts:â€‰A molecularâ€dynamics simulation. Journal of Chemical Physics, 1990, 92, 5057-5086.	3.0	3,331
2	Molecular dynamics simulation for polymers in the presence of a heat bath. Physical Review A, 1986, 33, 3628-3631.	2.5	1,532
3	Rheology and Microscopic Topology of Entangled Polymeric Liquids. Science, 2004, 303, 823-826.	12.6	670
4	Phase diagram and dynamics of Yukawa systems. Journal of Chemical Physics, 1988, 88, 3286-3312.	3.0	635
5	Equilibration of long chain polymer melts in computer simulations. Journal of Chemical Physics, 2003, 119, 12718-12728.	3.0	465
6	Structure of grafted polymeric brushes in solvents of varying quality: a molecular dynamics study. Macromolecules, 1993, 26, 3108-3117.	4.8	339
7	Structure of a grafted polymer brush: a molecular dynamics simulation. Macromolecules, 1989, 22, 4054-4059.	4.8	311
8	Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Statics. Journal of Chemical Physics, 2011, 134, 204904.	3.0	284
9	Osmotic pressure and viscoelastic shear moduli of concentrated emulsions. Physical Review E, 1997, 56, 3150-3166.	2.1	275
10	First-principles and classical molecular dynamics simulation of shocked polymers. Physical Review B, 2010, 81, .	3.2	261
11	Identifying the primitive path mesh in entangled polymer liquids. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 917-933.	2.1	223
12	Viscosity calculations ofn-alkanes by equilibrium molecular dynamics. Journal of Chemical Physics, 1997, 106, 9327-9336.	3.0	213
13	Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. II. Dynamics. Journal of Chemical Physics, 2011, 134, 204905.	3.0	210
14	Rheology of Ring Polymer Melts: From Linear Contaminants to Ring-Linear Blends. Physical Review Letters, 2012, 108, 038301.	7.8	179
15	Structure and relaxation of endâ€linked polymer networks. Journal of Chemical Physics, 1994, 101, 8169-8192.	3.0	170
16	Molecular dynamics of linear and branched alkanes. Journal of Chemical Physics, 1995, 103, 7156-7165.	3.0	164
17	Nanoparticle Diffusion in Polymer Nanocomposites. Physical Review Letters, 2014, 112, 108301.	7.8	157
18	Star Polymers: Experiment, Theory, and Simulation. Advances in Chemical Physics, 2007, , 67-163.	0.3	154

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19	Coarsening in the two-dimensional soap froth and the large-QPotts model: A detailed comparison. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1990, 62, 615-645.	0.6	148
20	Atomistic Simulations of End-Linked Poly(dimethylsiloxane) Networks:Â Structure and Relaxation. Macromolecules, 2004, 37, 3857-3864.	4.8	135
21	Capillary waves at liquid-vapor interfaces: A molecular dynamics simulation. Physical Review E, 1999, 60, 6708-6713.	2.1	127
22	Particle dynamics modeling methods for colloid suspensions. Computational Particle Mechanics, 2014, 1, 321-356.	3.0	124
23	Universal Viscosity Behavior of Polymer Nanocomposites. Physical Review Letters, 2012, 109, 198301.	7.8	123
24	Dynamics of n-alkanes: Comparison to Rouse model. Journal of Chemical Physics, 1998, 109, 798-805.	3.0	119
25	Statics and Dynamics of Symmetric Diblock Copolymers:Â A Molecular Dynamics Study. Macromolecules, 1999, 32, 595-609.	4.8	119
26	End grafted polymernanoparticles in a polymeric matrix: Effect of coverage and curvature. Soft Matter, 2011, 7, 1418-1425.	2.7	109
27	Grafted polymer brushes in polymeric matrices. Journal of Chemical Physics, 1996, 105, 5532-5541.	3.0	106
28	Spontaneous Asymmetry of Coated Spherical Nanoparticles in Solution and at Liquid-Vapor Interfaces. Physical Review Letters, 2010, 104, 235501.	7.8	106
29	Effective interactions between grafted nanoparticles in a polymer matrix. Soft Matter, 2012, 8, 5002.	2.7	104
30	Evaporation of Lennard-Jones fluids. Journal of Chemical Physics, 2011, 134, 224704.	3.0	96
31	Dispersing Nanoparticles in a Polymer Film via Solvent Evaporation. ACS Macro Letters, 2016, 5, 694-698.	4.8	95
32	Stress Relaxation in Entangled Polymer Melts. Physical Review Letters, 2010, 105, 068301.	7.8	94
33	Precursor Film Controlled Wetting of Pb on Cu. Physical Review Letters, 2003, 91, 236102.	7.8	86
34	Resolving Dynamic Properties of Polymers through Coarse-Grained Computational Studies. Physical Review Letters, 2016, 116, 058302.	7.8	85
35	Viscoelasticity and primitive path analysis of entangled polymer liquids: From F-actin to polyethylene. Journal of Chemical Physics, 2008, 128, 044902.	3.0	81
36	Structure and diffusion of nanoparticle monolayers floating at liquid/vapor interfaces: A molecular dynamics study. Journal of Chemical Physics, 2012, 136, 214702.	3.0	78

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37	Rouse mode analysis of chain relaxation in polymer nanocomposites. Soft Matter, 2015, 11, 4123-4132.	2.7	72
38	Dissolutive wetting of Ag on Cu: A molecular dynamics simulation study. Acta Materialia, 2005, 53, 3163-3177.	7.9	71
39	Stressâ€“strain relation of entangled polymer networks. Journal of Non-Crystalline Solids, 2000, 274, 139-146.	3.1	70
40	Accurate and efficient methods for modeling colloidal mixtures in an explicit solvent using molecular dynamics. Computer Physics Communications, 2008, 179, 320-329.	7.5	70
41	Entanglements of an End-Grafted Polymer Brush in a Polymeric Matrix. Macromolecules, 2007, 40, 8389-8395.	4.8	68
42	Intracrystalline Diffusion of Linear and Branched Alkanes in the Zeolites TON, EUO, and MFI. Journal of Physical Chemistry B, 1999, 103, 4949-4959.	2.6	66
43	Communication: Polymer entanglement dynamics: Role of attractive interactions. Journal of Chemical Physics, 2016, 145, 141101.	3.0	61
44	Nanoparticle Motion in Entangled Melts of Linear and Nonconcatenated Ring Polymers. Macromolecules, 2017, 50, 1749-1754.	4.8	61
45	Surface Wetting of Liquid Nanodroplets: Droplet-Size Effects. Physical Review Letters, 2005, 95, 107801.	7.8	60
46	Excluded-Volume Effects in Polymer Solutions. 2. Comparison of Experimental Results with Numerical Simulation Data. Macromolecules, 1999, 32, 3510-3517.	4.8	59
47	Tensile Fracture of Welded Polymer Interfaces: Miscibility, Entanglements, and Crazing. Macromolecules, 2014, 47, 6982-6989.	4.8	59
48	Molecular dynamics simulation of solventâ€“polymer interdiffusion: Fickian diffusion. Journal of Chemical Physics, 2004, 120, 2989-2995.	3.0	57
49	Molecular dynamics simulations of evaporation-induced nanoparticle assembly. Journal of Chemical Physics, 2013, 138, 064701.	3.0	54
50	Effects of Functional Groups and Ionization on the Structure of Alkanethiol-Coated Gold Nanoparticles. Langmuir, 2014, 30, 11075-11085.	3.5	54
51	Rouse Mode Analysis of Chain Relaxation in Homopolymer Melts. Macromolecules, 2014, 47, 6925-6931.	4.8	54
52	Strain-Dependent Localization, Microscopic Deformations, and Macroscopic Normal Tensions in Model Polymer Networks. Physical Review Letters, 2004, 93, 257801.	7.8	53
53	Forces between functionalized silica nanoparticles in solution. Physical Review E, 2009, 79, 050501.	2.1	53
54	Topological Linking Drives Anomalous Thickening of Ring Polymers in Weak Extensional Flows. Physical Review Letters, 2020, 124, 027801.	7.8	53

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55	Effect of particle shape and charge on bulk rheology of nanoparticle suspensions. Journal of Chemical Physics, 2010, 132, .	3.0	52
56	Nonlinear Shear Rheology of Entangled Polymer Rings. Macromolecules, 2021, 54, 2811-2827.	4.8	51
57	Permanent Set of Cross-Linking Networks:Â Comparison of Theory with Molecular Dynamics Simulations. Macromolecules, 2006, 39, 5521-5530.	4.8	50
58	Connectivity and Entanglement Stress Contributions in Strained Polymer Networks. Macromolecules, 2008, 41, 4920-4928.	4.8	50
59	Healing of polymer interfaces: Interfacial dynamics, entanglements, and strength. Physical Review E, 2014, 90, 012602.	2.1	50
60	Water in Nanoconfinement between Hydrophilic Self-Assembled Monolayers. Langmuir, 2008, 24, 5209-5212.	3.5	49
61	Coarse-Grained Modeling of Polyethylene Melts: Effect on Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2890-2896.	5.3	47
62	Simulating the miscibility of nanoparticles and polymer melts. Soft Matter, 2013, 9, 5417.	2.7	46
63	Stratification in Drying Films Containing Bidisperse Mixtures of Nanoparticles. Langmuir, 2018, 34, 7161-7170.	3.5	44
64	Influence of intracrystalline diffusion in shape selective catalytic test reactions. Catalysis Letters, 1998, 56, 95-104.	2.6	43
65	Effect of shape and friction on the packing and flow of granular materials. Physical Review E, 2018, 98, .	2.1	42
66	Molecular Dynamics Simulations of the Force between a Polymer Brush and an AFM Tip. Macromolecules, 1996, 29, 8282-8284.	4.8	40
67	Molecular dynamics of linear and branched alkanes: Simulations and nuclear magnetic resonance results. Journal of Chemical Physics, 1996, 105, 5208-5215.	3.0	40
68	Mesoscale hydrodynamics via stochastic rotation dynamics: Comparison with Lennard-Jones fluid. Journal of Chemical Physics, 2010, 132, 174106.	3.0	40
69	Anomalous mixing behavior of polyisobutylene/polypropylene blends: Molecular dynamics simulation study. Journal of Chemical Physics, 2004, 120, 8883-8886.	3.0	36
70	Entangled polymer systems. Computer Physics Communications, 2005, 169, 75-81.	7.5	36
71	Threadingâ€“Unthreading Transition of Linear-Ring Polymer Blends in Extensional Flow. ACS Macro Letters, 2020, 9, 1452-1457.	4.8	36
72	Molecular dynamics simulations of reactive wetting. Scripta Materialia, 2002, 47, 393-398.	5.2	34

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73	Assembly of responsive-shape coated nanoparticles at water surfaces. Nanoscale, 2014, 6, 5132.	5.6	34
74	Nanorheology of Entangled Polymer Melts. Physical Review Letters, 2018, 120, 057801.	7.8	34
75	Fully Atomistic Simulations of the Response of Silica Nanoparticle Coatings to Alkane Solvents. Langmuir, 2012, 28, 17443-17449.	3.5	33
76	Surface-tethered chains entangled in a polymer melt: Effects on adhesion dynamics. Physical Review E, 2001, 64, 050802.	2.1	32
77	High Strength, Molecularly Thin Nanoparticle Membranes. Physical Review Letters, 2014, 113, 258301.	7.8	31
78	Superfast assembly and synthesis of gold nanostructures using nanosecond low-temperature compression via magnetic pulsed power. Nature Communications, 2017, 8, 14778.	12.8	31
79	Granular packings with sliding, rolling, and twisting friction. Physical Review E, 2020, 102, 032903.	2.1	31
80	Effective potentials between nanoparticles in suspension. Journal of Chemical Physics, 2011, 134, 144902.	3.0	28
81	No-slip boundary conditions and forced flow in multiparticle collision dynamics. Physical Review E, 2012, 86, 066703.	2.1	28
82	Coating thickness and coverage effects on the forces between silica nanoparticles in water. Journal of Chemical Physics, 2014, 140, 194904.	3.0	28
83	Liquid Nanodroplets Spreading on Chemically Patterned Surfaces. Langmuir, 2006, 22, 4745-4749.	3.5	27
84	Crazing of nanocomposites with polymer-tethered nanoparticles. Journal of Chemical Physics, 2016, 145, 094902.	3.0	27
85	Dynamics of linear and branched alkane melts: Molecular dynamics test of theory for long time dynamics. Journal of Chemical Physics, 1998, 108, 9155-9167.	3.0	25
86	Shear thinning of nanoparticle suspensions. Physical Review E, 2009, 79, 021401.	2.1	24
87	Clustering effects in ionic polymers: Molecular dynamics simulations. Physical Review E, 2015, 92, 022601.	2.1	24
88	Stratification of drying particle suspensions: Comparison of implicit and explicit solvent simulations. Journal of Chemical Physics, 2019, 150, 224901.	3.0	24
89	Flow-Arrest Transitions in Frictional Granular Matter. Physical Review Letters, 2019, 122, 048003.	7.8	23
90	Dynamics in entangled polyethylene melts. European Physical Journal: Special Topics, 2016, 225, 1707-1722.	2.6	22

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91	Effects of Tethered Polymers on Dynamics of Nanoparticles in Unentangled Polymer Melts. Macromolecules, 2020, 53, 6898-6906.	4.8	20
92	Diffusion of Thin Nanorods in Polymer Melts. Macromolecules, 2021, 54, 7051-7059.	4.8	20
93	Composite entanglement topology and extensional rheology of symmetric ring-linear polymer blends. Journal of Rheology, 2022, 66, 49-65.	2.6	20
94	Entanglement effects in model polymer networks. Macromolecular Symposia, 1995, 93, 53-67.	0.7	19
95	Conformational study of a single molecule of poly para phenylene ethynylenes in dilute solutions. Journal of Chemical Physics, 2011, 134, 244906.	3.0	19
96	Ligand structure and mechanical properties of single-nanoparticle-thick membranes. Physical Review E, 2015, 91, 062403.	2.1	19
97	Effect of Chain Length Dispersity on the Mobility of Entangled Polymers. Physical Review Letters, 2018, 121, 057802.	7.8	19
98	High temperature wetting: Insights from atomistic simulations. Current Opinion in Solid State and Materials Science, 2005, 9, 174-180.	11.5	17
99	Liquid-vapor coexistence for nanoparticles of various size. Journal of Chemical Physics, 2008, 129, 164504.	3.0	17
100	Cluster Morphology-Polymer Dynamics Correlations in Sulfonated Polystyrene Melts: Computational Study. Physical Review Letters, 2016, 116, 158001.	7.8	17
101	Control of Stratification in Drying Particle Suspensions via Temperature Gradients. Langmuir, 2019, 35, 4296-4304.	3.5	17
102	Ordering nanoparticles with polymer brushes. Journal of Chemical Physics, 2017, 147, 224901.	3.0	16
103	Assembly of Polymer-Grafted Nanoparticles in Polymer Matrices. ACS Nano, 2020, 14, 13491-13499.	14.6	16
104	Shear rheology of extended nanoparticles. Physical Review E, 2010, 82, 010201.	2.1	13
105	Internal Correlations and Stability of Polydots, Soft Conjugated Polymeric Nanoparticles. ACS Macro Letters, 2013, 2, 700-704.	4.8	13
106	Polymer Topology Effects on Dynamics of Comb Polymer Melts. Macromolecules, 2018, 51, 7621-7628.	4.8	13
107	Viscometric flow of dense granular materials under controlled pressure and shear stress. Journal of Fluid Mechanics, 2021, 907, .	3.4	13
108	Superstretchable Elastomer from Cross-linked Ring Polymers. Physical Review Letters, 2022, 128, .	7.8	13

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109	Temperature effects on nanostructure and mechanical properties of single-nanoparticle thick membranes. Faraday Discussions, 2015, 181, 339-354.	3.2	12
110	Association of a multifunctional ionic block copolymer in a selective solvent. Journal of Chemical Physics, 2016, 145, 184903.	3.0	12
111	Mechanics of Gold Nanoparticle Superlattices at High Hydrostatic Pressures. Journal of Physical Chemistry C, 2019, 123, 17530-17538.	3.1	11
112	Brush-Like Polymers and Entanglements: From Linear Chains to Filaments. ACS Macro Letters, 2019, 8, 1328-1333.	4.8	11
113	Polymers at Liquid/Vapor Interface. ACS Macro Letters, 2017, 6, 1191-1195.	4.8	10
114	Jamming of bidisperse frictional spheres. Physical Review Research, 2021, 3, .	3.6	10
115	Temperature dependence of domain growth. Journal of Applied Physics, 1984, 55, 2432-2434.	2.5	9
116	Structure of Rigid Polymers Confined to Nanoparticles: Molecular Dynamics Simulations Insight. Langmuir, 2016, 32, 2102-2109.	3.5	9
117	Diverse Spreading Behavior of Binary Polymer Nanodroplets. Langmuir, 2005, 21, 7959-7963.	3.5	8
118	Structured Ionomer Thin Films at Water Interface: Molecular Dynamics Simulation Insight. Langmuir, 2017, 33, 11070-11076.	3.5	8
119	Conformation of ionizable poly Para phenylene ethynylene in dilute solutions. Journal of Polymer Science, Part B: Polymer Physics, 2016, 54, 582-588.	2.1	7
120	Effects of interaction strength of associating groups on linear and star polymer dynamics. Journal of Chemical Physics, 2021, 154, 074903.	3.0	7
121	Nonlinear Elongation Flows in Associating Polymer Melts: From Homogeneous to Heterogeneous Flow. Physical Review X, 2022, 12, .	8.9	7
122	Irreversibility of infinite range spin glasses. Journal of Applied Physics, 1984, 55, 1661-1663.	2.5	6
123	Phase Behavior of a Single Structured Ionomer Chain in Solution. Macromolecular Theory and Simulations, 2014, 23, 543-549.	1.4	6
124	Dynamics of Polydots: Soft Luminescent Polymeric Nanoparticles. Macromolecules, 2016, 49, 2399-2407.	4.8	6
125	Structure and Dynamics of Ionic Block Copolymer Melts: Computational Study. Macromolecules, 2017, 50, 7388-7398.	4.8	6
126	Effects of Ionic Group Distribution on the Structure and Dynamics of Amorphous Polymer Melts. Macromolecules, 2022, 55, 217-223.	4.8	6

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127	Viscoelastic Response of Dispersed Entangled Polymer Melts. Macromolecules, 2020, 53, 8400-8405.	4.8	5
128	Evolution of internal granular structure at the flow-arrest transition. Granular Matter, 2020, 22, 1.	2.2	5
129	Overlap Concentration in Salt-Free Polyelectrolyte Solutions. Macromolecules, 2021, 54, 10068-10073.	4.8	5
130	Flow and arrest in stressed granular materials. Soft Matter, 2022, 18, 735-743.	2.7	5
131	Shear Is Not Always Simple: Rate-Dependent Effects of Flow Type on Granular Rheology. Physical Review Letters, 2021, 127, 268003.	7.8	5
132	Solvent controlled ion association in structured copolymers: Molecular dynamics simulations in dilute solutions. Journal of Chemical Physics, 2015, 143, 124905.	3.0	4
133	Soft nanoparticles: nano ionic networks of associated ionic polymers. Nanoscale, 2017, 9, 2117-2122.	5.6	4
134	Modeling pressure-driven assembly of polymer coated nanoparticles. AIP Conference Proceedings, 2018, , .	0.4	4
135	Resolving Properties of Entangled Polymers Melts Through Atomistic Derived Coarse-Grained Models. , 2020, , 1397-1410.		4
136	Coarsening in Two-Dimensional Soap Froths and the Large-Q Potts Model. Materials Research Society Symposia Proceedings, 1991, 237, 101.	0.1	3
137	End-anchored polymers in good solvents from the single chain limit to high anchoring densities. Journal of Chemical Physics, 2016, 145, 174904.	3.0	3
138	Overlap Concentration of Sodium Polystyrene Sulfonate in Solution. ACS Macro Letters, 2022, 11, 217-222.	4.8	3
139	Luminescent tunable polydots: Charge effects in confined geometry. Journal of Chemical Physics, 2017, 146, 244907.	3.0	2
140	Monte Carlo Simulations of the Chemical Potential and Free Energy for Trimer and Hexamer Rings. Molecular Simulation, 1989, 2, 69-88.	2.0	1
141	Temperature response of soft ionizable polymer nanoparticles. Journal of Chemical Physics, 2018, 149, 084903.	3.0	1
142	Stress Relaxation of Comb Polymer Melts. Tribology Letters, 2021, 69, 1.	2.6	1
143	What can we Learn from Molecular Dynamics Simulations of Macromolecular Liquids?. Materials Research Society Symposia Proceedings, 1989, 177, 77.	0.1	0
144	Simulations of Polymer Blends and Interfaces. Materials Research Society Symposia Proceedings, 1996, 461, 129.	0.1	0

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145	Simulations of Lubricants in Confined Geometries. Materials Research Society Symposia Proceedings, 1996, 464, 65.	0.1	0
146	Resolving Properties of Entangled Polymers Melts Through Atomistic Derived Coarse-Grained Models. , 2018, , 1-14.		0
147	Interfacial Response and Structural Adaptation of Structured Polyelectrolyte Thin Films. Macromolecules, 2021, 54, 2892-2898.	4.8	0