

Nikos Ch Karayiannis

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.

47
papers

1,645
citations

23
h-index

40
g-index

50
ext. papers

1,807
ext. citations

4.1
avg, IF

4.64
L-index

#	Paper	IF	Citations
47	Crystal, Fivefold and Glass Formation in Clusters of Polymers Interacting with the Square Well Potential. <i>Polymers</i> , 2020 , 12,	4.5	4
46	Identification of Local Structure in 2-D and 3-D Atomic Systems through Crystallographic Analysis. <i>Crystals</i> , 2020 , 10, 1008	2.3	0
45	Self-Avoiding Random Walks as a Model to Study Athermal Linear Polymers under Extreme Plate Confinement. <i>Polymers</i> , 2020 , 12,	4.5	2
44	Effect of Bond Tangency/Gap on the Crystallization of Athermal Polymer Packings. <i>Proceedings (mdpi)</i> , 2018 , 2, 63	0.3	
43	Absorption 2018 , 1-115		0
42	Confined Polymers as Self-Avoiding Random Walks on Restricted Lattices. <i>Polymers</i> , 2018 , 10,	4.5	3
41	Off-lattice simulation algorithms for athermal chain molecules under extreme confinement. <i>Journal of Computational Physics</i> , 2018 , 375, 918-934	4.1	11
40	i-Rheo GT: Transforming from Time to Frequency Domain without Artifacts. <i>Macromolecules</i> , 2018 , 51, 5055-5068	5.5	17
39	The role of bond tangency and bond gap in hard sphere crystallization of chains. <i>Soft Matter</i> , 2015 , 11, 1688-700	3.6	14
38	Monte Carlo simulations of densely-packed athermal polymers in the bulk and under confinement. <i>Chemical Engineering Science</i> , 2015 , 121, 118-132	4.4	9
37	Effect of chain stiffness on the competition between crystallization and glass-formation in model unentangled polymers. <i>Journal of Chemical Physics</i> , 2015 , 143, 144901	3.9	18
36	Twinning of Polymer Crystals Suppressed by Entropy. <i>Symmetry</i> , 2014 , 6, 758-780	2.7	6
35	A metric to gauge local distortion in metallic glasses and supercooled liquids. <i>Acta Materialia</i> , 2014 , 72, 229-238	8.4	8
34	Jamming and crystallization in athermal polymer packings. <i>Philosophical Magazine</i> , 2013 , 93, 4108-4131	1.6	11
33	Simple model for chain packing and crystallization of soft colloidal polymers. <i>Physical Review E</i> , 2013 , 88, 012601	2.4	22
32	Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings. <i>Soft Matter</i> , 2012 , 8, 844-858	3.6	38
31	Spontaneous crystallization in athermal polymer packings. <i>International Journal of Molecular Sciences</i> , 2012 , 14, 332-58	6.3	21

30	Influence of Nanorod Inclusions on Structure and Primitive Path Network of Polymer Nanocomposites at Equilibrium and Under Deformation. <i>Macromolecules</i> , 2011 , 44, 1034-1045	5.5	83
29	Fivefold symmetry as an inhibitor to hard-sphere crystallization. <i>Physical Review E</i> , 2011 , 83, 061505	2.4	38
28	Modeling of crystal nucleation and growth in athermal polymers: self-assembly of layered nano-morphologies. <i>Soft Matter</i> , 2010 , 6, 2160	3.6	35
27	Entropy-driven crystallization in dense systems of athermal chain molecules. <i>Physical Review Letters</i> , 2009 , 103, 045703	7.4	44
26	The characteristic crystallographic element norm: A descriptor of local structure in atomistic and particulate systems. <i>Journal of Chemical Physics</i> , 2009 , 130, 074704	3.9	30
25	Combined molecular algorithms for the generation, equilibration and topological analysis of entangled polymers: methodology and performance. <i>International Journal of Molecular Sciences</i> , 2009 , 10, 5054-89	6.3	124
24	Computer simulations of amorphous polymers: From quantum mechanical calculations to mesoscopic models. <i>Computational and Theoretical Chemistry</i> , 2009 , 898, 62-72		10
23	Detailed atomistic molecular dynamics simulations of alpha-conotoxin AuIB in water. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 5016-24	3.4	7
22	Structure, dimensions, and entanglement statistics of long linear polyethylene chains. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 442-55	3.4	56
21	Contact network in nearly jammed disordered packings of hard-sphere chains. <i>Physical Review E</i> , 2009 , 80, 011307	2.4	29
20	Random packing of model polymers: local structure, topological hindrance and universal scaling. <i>Soft Matter</i> , 2009 , 5, 1762	3.6	40
19	The structure of random packings of freely jointed chains of tangent hard spheres. <i>Journal of Chemical Physics</i> , 2009 , 130, 164908	3.9	41
18	Dense and nearly jammed random packings of freely jointed chains of tangent hard spheres. <i>Physical Review Letters</i> , 2008 , 100, 050602	7.4	46
17	Monte Carlo Scheme for Generation and Relaxation of Dense and Nearly Jammed Random Structures of Freely Jointed Hard-Sphere Chains. <i>Macromolecules</i> , 2008 , 41, 1537-1551	5.5	37
16	Molecular simulation of the effect of temperature and architecture on polyethylene barrier properties. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 5646-60	3.4	25
15	Flexible chain molecules in the marginal and concentrated regimes: universal static scaling laws and cross-over predictions. <i>Journal of Chemical Physics</i> , 2008 , 128, 174901	3.9	23
14	Universal scaling, entanglements, and knots of model chain molecules. <i>Physical Review Letters</i> , 2008 , 101, 265702	7.4	44
13	Min-map bias Monte Carlo for chain molecules: biased Monte Carlo sampling based on bijective minimum-to-minimum mapping. <i>Journal of Chemical Physics</i> , 2006 , 125, 164108	3.9	10

12	Structural design of polymers for membrane based separation processes using reverse simulation approach. <i>Computer Aided Chemical Engineering</i> , 2006 , 21, 689-694	0.6	1
11	Primitive Path Identification and Entanglement Statistics in Polymer Melts: Results from Direct Topological Analysis on Atomistic Polyethylene Models. <i>Macromolecules</i> , 2006 , 39, 4207-4216	5.5	137
10	Atomistic Molecular Dynamics simulation of short-chain branched polyethylene melts. <i>Computer Aided Chemical Engineering</i> , 2006 , 22, 333-357	0.6	
9	Detailed Atomistic Simulation of the Barrier Properties of Linear and Short-Chain Branched Polyethylene Melts Through a Hierarchical Modeling Approach. <i>Computer Aided Chemical Engineering</i> , 2006 , 201-239	0.6	
8	Advanced Monte Carlo Methods for the atomistic simulation of polymers with a linear or a non-linear molecular architecture. <i>Computer Aided Chemical Engineering</i> , 2006 , 31-67	0.6	2
7	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. <i>Macromolecules</i> , 2005 , 38, 7134-7149	5.5	47
6	Hierarchical Modeling of the Dynamics of Polymers with a Nonlinear Molecular Architecture: Calculation of Branch Point Friction and Chain Reptation Time of H-Shaped Polyethylene Melts from Long Molecular Dynamics Simulations. <i>Macromolecules</i> , 2005 , 38, 8583-8596	5.5	52
5	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). <i>Macromolecules</i> , 2004 , 37, 2978-2995	5.5	95
4	An advanced Monte Carlo method for the equilibration of model long-chain branched polymers with a well-defined molecular architecture: Detailed atomistic simulation of an H-shaped polyethylene melt. <i>Journal of Chemical Physics</i> , 2003 , 118, 2451	3.9	41
3	A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture. <i>Physical Review Letters</i> , 2002 , 88, 105503	7.4	200
2	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. <i>Journal of Chemical Physics</i> , 2002 , 117, 5465-5479	3.9	117
1	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. <i>Chemical Engineering Science</i> , 2001 , 56, 2789-2801	4.4	42