Nikos Ch Karayiannis

List of Publications by Citations

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	A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture. *Physical Review Letters*, **2002**, 88, 105503	7.4	200
46	Primitive Path Identification and Entanglement Statistics in Polymer Melts: Results from Direct Topological Analysis on Atomistic Polyethylene Models. *Macromolecules*, **2006**, 39, 4207-4216	5.5	137
45	Combined molecular algorithms for the generation, equilibration and topological analysis of entangled polymers: methodology and performance. *International Journal of Molecular Sciences*, **2009**, 10, 5054-89	6.3	124
44	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. *Journal of Chemical Physics*, **2002**, 117, 5465-5479	3.9	117
43	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). *Macromolecules*, **2004**, 37, 2978-2995	5.5	95
42	Influence of Nanorod Inclusions on Structure and Primitive Path Network of Polymer Nanocomposites at Equilibrium and Under Deformation. *Macromolecules*, **2011**, 44, 1034-1045	5.5	83
41	Structure, dimensions, and entanglement statistics of long linear polyethylene chains. *Journal of Physical Chemistry B*, **2009**, 113, 442-55	3.4	56
40	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. *Macromolecules*, **2005**, 38, 8583-8596	5.5	52
39	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. *Macromolecules*, **2005**, 38, 7134-7149	5.5	47
38	Dense and nearly jammed random packings of freely jointed chains of tangent hard spheres. *Physical Review Letters*, **2008**, 100, 050602	7.4	46
37	Entropy-driven crystallization in dense systems of athermal chain molecules. *Physical Review Letters* , **2009**, 103, 045703	7.4	44
36	Universal scaling, entanglements, and knots of model chain molecules. *Physical Review Letters*, **2008**, 101, 265702	7.4	44
35	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. *Chemical Engineering Science*, **2001**, 56, 2789-2801	4.4	42
34	The structure of random packings of freely jointed chains of tangent hard spheres. *Journal of Chemical Physics*, **2009**, 130, 164908	3.9	41
33	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. *Journal of Chemical Physics*, **2003**, 118, 2451	3.9	41
32	Random packing of model polymers: local structure, topological hindrance and universal scaling. *Soft Matter*, **2009**, 5, 1762	3.6	40
31	Evolution of fivefold local symmetry during crystal nucleation and growth in dense hard-sphere packings. *Soft Matter*, **2012**, 8, 844-858	3.6	38

30	Fivefold symmetry as an inhibitor to hard-sphere crystallization. *Physical Review E*, **2011**, 83, 061505	2.4	38
29	Monte Carlo Scheme for Generation and Relaxation of Dense and Nearly Jammed Random Structures of Freely Jointed Hard-Sphere Chains. *Macromolecules*, **2008**, 41, 1537-1551	5.5	37
28	Modeling of crystal nucleation and growth in athermal polymers: self-assembly of layered nano-morphologies. *Soft Matter*, **2010**, 6, 2160	3.6	35
27	The characteristic crystallographic element norm: A descriptor of local structure in atomistic and particulate systems. *Journal of Chemical Physics*, **2009**, 130, 074704	3.9	30
26	Contact network in nearly jammed disordered packings of hard-sphere chains. *Physical Review E*, **2009**, 80, 011307	2.4	29
25	Molecular simulation of the effect of temperature and architecture on polyethylene barrier properties. *Journal of Physical Chemistry B*, **2008**, 112, 5646-60	3.4	25
24	Flexible chain molecules in the marginal and concentrated regimes: universal static scaling laws and cross-over predictions. *Journal of Chemical Physics*, **2008**, 128, 174901	3.9	23
23	Simple model for chain packing and crystallization of soft colloidal polymers. *Physical Review E*, **2013**, 88, 012601	2.4	22
22	Spontaneous crystallization in athermal polymer packings. *International Journal of Molecular Sciences*, **2012**, 14, 332-58	6.3	21
21	Effect of chain stiffness on the competition between crystallization and glass-formation in model unentangled polymers. *Journal of Chemical Physics*, **2015**, 143, 144901	3.9	18
20	i-Rheo GT: Transforming from Time to Frequency Domain without Artifacts. *Macromolecules*, **2018**, 51, 5055-5068	5.5	17
19	The role of bond tangency and bond gap in hard sphere crystallization of chains. *Soft Matter*, **2015**, 11, 1688-700	3.6	14
18	Jamming and crystallization in athermal polymer packings. *Philosophical Magazine*, **2013**, 93, 4108-4131	1.6	11
17	Off-lattice simulation algorithms for athermal chain molecules under extreme confinement. *Journal of Computational Physics*, **2018**, 375, 918-934	4.1	11
16	Computer simulations of amorphous polymers: From quantum mechanical calculations to mesoscopic models. *Computational and Theoretical Chemistry*, **2009**, 898, 62-72		10
15	Min-map bias Monte Carlo for chain molecules: biased Monte Carlo sampling based on bijective minimum-to-minimum mapping. *Journal of Chemical Physics*, **2006**, 125, 164108	3.9	10
14	Monte Carlo simulations of densely-packed athermal polymers in the bulk and under confinement. *Chemical Engineering Science*, **2015**, 121, 118-132	4.4	9
13	A metric to gauge local distortion in metallic glasses and supercooled liquids. *Acta Materialia*, **2014**, 72, 229-238	8.4	8

12	Detailed atomistic molecular dynamics simulations of alpha-conotoxin AuIB in water. *Journal of Physical Chemistry B*, **2009**, 113, 5016-24	3.4	7
11	Twinning of Polymer Crystals Suppressed by Entropy. *Symmetry*, **2014**, 6, 758-780	2.7	6
10	Crystal, Fivefold and Glass Formation in Clusters of Polymers Interacting with the Square Well Potential. *Polymers*, **2020**, 12,	4.5	4
9	Confined Polymers as Self-Avoiding Random Walks on Restricted Lattices. *Polymers*, **2018**, 10,	4.5	3
8	Advanced Monte Carlo Methods for the atomistic simulation of polymers with a linear or a non-linear molecular architecture. *Computer Aided Chemical Engineering*, **2006**, 31-67	0.6	2
7	Self-Avoiding Random Walks as a Model to Study Athermal Linear Polymers under Extreme Plate Confinement. *Polymers*, **2020**, 12,	4.5	2
6	Structural design of polymers for membrane based separation processes using reverse simulation approach. *Computer Aided Chemical Engineering*, **2006**, 21, 689-694	0.6	1
5	Identification of Local Structure in 2-D and 3-D Atomic Systems through Crystallographic Analysis. *Crystals*, **2020**, 10, 1008	2.3	0
4	Absorption **2018**, 1-115		0
3	Effect of Bond Tangency/Gap on the Crystallization of Athermal Polymer Packings. *Proceedings (mdpi)*, **2018**, 2, 63	0.3	
2	Atomistic Molecular Dynamics simulation of short□chain branched polyethylene melts. *Computer Aided Chemical Engineering*, **2006**, 22, 333-357	0.6	
1	Detailed Atomistic Simulation of the Barrier Properties of Linear and Short□Chain Branched Polyethylene Melts Through a Hierarchical Modeling Approach. *Computer Aided Chemical Engineering*, **2006**, 201-239	0.6	