Konstantinos Karatasos

List of Publications by Year
in descending order

71 papers	1,985 citations	236833 25 h-index	254106 43 g-index
72 all docs	72 docs citations	72 times ranked	1859 citing authors

#	Article	IF	Citations
1	Molecular Dynamics Simulations of Essential Oil Ingredients Associated with Hyperbranched Polymer Drug Carriers. Polymers, 2022, 14, 1762.	2.0	1
2	Molecular dynamics simulations of hyperbranched poly(ethylene imine)â€“graphene oxide nanocomposites as dye adsorbents for water purification. Physical Chemistry Chemical Physics, 2021, 23, 22874-22884.	1.3	13
3	Effect of Nanofiller Size on the Mechanical Properties of Poly(acrylic acid)/Graphene Oxide Nanocomposites. Macromolecules, 2021, 54, 4164-4175.	2.2	7
4	Multiscale Modeling Examples: New Polyelectrolyte Nanocomposite Membranes for Perspective Fuel Cells and Flow Batteries. Springer Series in Materials Science, 2021, , 133-177.	0.4	1
5	Bound Layer Polymer Behavior on Graphene and Graphene Oxide Nanosheets. Macromolecules, 2020, 53, 6190-6203.	2.2	10
6	Liposome-Templated Indocyanine Green J- Aggregates for In Vivo Near Infrared Imaging and Stable Photothermal Heating. Nanotheranostics, 2020, 4, 91-106.	2.7	36
7	Complexation of single stranded RNA with an ionizable lipid: an all-atom molecular dynamics simulation study. Soft Matter, 2020, 16, 6993-7005.	1.2	23
8	Molecular Dynamics Simulations of Hydrated Poly(amidoamine) Dendrimer/Graphene Oxide Nanocomposite Membranes. Journal of Physical Chemistry C, 2020, 124, 9512-9522.	1.5	6
9	Computational Study of the Interaction of a PEGylated Hyperbranched Polymer/Doxorubicin Complex with a Bilipid Membrane. Fluids, 2019, 4, 17.	0.8	4
10	Molecular Dynamics Simulation of the Capillary Leveling of a Glass-Forming Liquid. Journal of Physical Chemistry B, 2019, 123, 8543-8549.	1.2	4
11	A microscopic view of graphene-oxide/poly(acrylic acid) physical hydrogels: effects of polymer charge and graphene oxide loading. Soft Matter, 2018, 14, 614-627.	1.2	18
12	Effects of the fillerâ€™s loading in features of poly(acrylic acid)/graphene oxide nanocomposites. Materials Today: Proceedings, 2018, 5, 27526-27535.	0.9	2
13	Nanostructure and Dynamics of Humidified Nafion/Graphene-Oxide Composites via Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2018, 122, 22864-22875.	1.5	16
14	Novel polyelectrolyte membranes for fuel and flow batteries: Insights from simulations. AIP Conference Proceedings, 2018, , .	0.3	2
15	Temperature dependence of dynamic and mechanical properties in poly(acrylic acid)/graphene oxide nanocomposites. Materials Today Communications, 2017, 13, 359-366.	0.9	14
16	Frequency Dependent Non- Thermal Effects of Oscillating Electric Fields in the Microwave Region on the Properties of a Solvated Lysozyme System: A Molecular Dynamics Study. PLoS ONE, 2017, 12, e0169505.	1.1	12
17	Characterization of a graphene oxide/poly(acrylic acid) nanocomposite by means of molecular dynamics simulations. RSC Advances, 2016, 6, 109267-109277.	1.7	20
18	Graphene/poly(ethylene glycol) nanocomposites as studied by molecular dynamics simulations. Materials and Design, 2016, 97, 163-174.	3.3	37

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19	Detailed study of the dielectric function of a lysozyme solution studied with molecular dynamics simulations. European Biophysics Journal, 2015, 44, 599-611.	1.2	7
20	Dynamics of dendritic polymers in the bulk and under confinement. , 2014, , .		0
21	Graphene/Hyperbranched Polymer Nanocomposites: Insight from Molecular Dynamics Simulations. Macromolecules, 2014, 47, 8833-8845.	2.2	28
22	Self-Association and Complexation of the Anti-Cancer Drug Doxorubicin with PEGylated Hyperbranched Polyesters in an Aqueous Environment. Journal of Physical Chemistry B, 2013, 117, 2564-2575.	1.2	21
23	Multiscale Modeling of Dendrimers and Dendrons for Drug and Nucleic Acid Delivery. , 2013, , 148-166.		1
24	Structure and Dynamics of Hyperbranched Polymer/Layered Silicate Nanocomposites. Macromolecules, 2013, 46, 2842-2855.	2.2	41
25	Complexes between Poly(amido amine) Dendrimers and Poly(methacrlyic acid): Insight from Molecular Dynamics Simulations. Macromolecular Symposia, 2013, 331-332, 34-42.	0.4	3
26	Modeling the formation of ordered nano-assemblies comprised by dendrimers and linear polyelectrolytes: The role of Coulombic interactions. Journal of Chemical Physics, 2012, 137, 144905.	1.2	5
27	Conformational Effects in Non-Stoichiometric Complexes of Two Hyperbranched Molecules with a Linear Polyelectrolyte. Polymers, 2012, 4, 240-255.	2.0	9
28	Chimeric advanced drug delivery nano systems (chi-aDDnSs) for shikonin combining dendritic and liposomal technology. International Journal of Pharmaceutics, 2012, 422, 381-389.	2.6	38
29	Poly(amidoamine)â€based Dendrimer/siRNA Complexation Studied by Computer Simulations: Effects of pH and Generation on Dendrimer Structure and siRNA Binding. Macromolecular Bioscience, 2012, 12, 225-240.	2.1	61
30	Tell Me Something I Do Not Know. Multiscale Molecular Modeling of Dendrimer/ Dendron Organization and Self-Assembly In Gene Therapy. Current Medicinal Chemistry, 2012, 19, 5062-5087.	1.2	28
31	Simulation of a Symmetric Binary Mixture of Charged Dendrimers Under Varying Electrostatic Interactions: Static and Dynamic Aspects. Macromolecules, 2011, 44, 6605-6614.	2.2	8
32	Modeling of hyperbranched polyesters as hosts for the multifunctional bioactive agent shikonin. Physical Chemistry Chemical Physics, 2011, 13, 10808.	1.3	16
33	Dynamics of counterions in dendrimer polyelectrolyte solutions. Journal of Chemical Physics, 2009, 130, 114903.	1.2	23
34	Investigation of thermodynamic properties of hyperbranched aliphatic polyesters by inverse gas chromatography. Journal of Chromatography A, 2009, 1216, 8979-8985.	1.8	32
35	Molecular Dynamics Simulations of a Hyperbranched Poly(ester amide): Statics, Dynamics, and Hydrogen Bonding. Journal of Physical Chemistry B, 2009, 113, 5356-5368.	1.2	36
36	Local Dynamics and Hydrogen Bonding in Hyperbranched Aliphatic Polyesters. Macromolecules, 2009, 42, 9581-9591.	2.2	26

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37	Association of a Weakly Acidic Anti-Inflammatory Drug (Ibuprofen) with a Poly(Amidoamine) Dendrimer as Studied by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 10984-10993.	1.2	79
38	Molecular dynamics simulations of polyamidoamine dendrimers and their complexes with linear poly(ethylene oxide) at different pH conditions: static properties and hydrogen bonding. Physical Chemistry Chemical Physics, 2009, 11, 10017.	1.3	46
39	Electrostaticallyâ€driven Ordering in Model Dendrimer Polyelectrolytes: Effects of Concentration. Macromolecular Symposia, 2009, 278, 32-39.	0.4	6
40	Brownian dynamics simulations of complexes of hyperbranched polymers with linear polyelectrolytes: Effects of the strength of electrostatic interactions on static properties. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2008, 152, 114-118.	1.7	8
41	Investigation of thermodynamic properties of hyperbranched poly(ester amide) by inverse gas chromatography. Journal of Polymer Science, Part B: Polymer Physics, 2008, 46, 2166-2172.	2.4	18
42	Structural effects in overcharging in complexes of hyperbranched polymers with linear polyelectrolytes. Soft Matter, 2008, 4, 453.	1.2	25
43	Shear-induced effects in hyperbranched-linear polyelectrolyte complexes. Journal of Chemical Physics, 2008, 129, 034901.	1.2	8
44	Self-Organization in Dendrimer Polyelectrolytes. Macromolecules, 2008, 41, 1025-1033.	2.2	30
45	Effects of topology and size on statics and dynamics of complexes of hyperbranched polymers with linear polyelectrolytes. Journal of Chemical Physics, 2007, 127, 214903.	1.2	24
46	Non-Gaussian nature of glassy dynamics by cage to cage motion. Physical Review E, 2007, 75, 011504.	0.8	66
47	Glass Transition in Dendrimers. Macromolecules, 2006, 39, 4619-4626.	2.2	28
48	Computational polymer dynamics via DL_POLY. Molecular Simulation, 2006, 32, 1017-1023.	0.9	0
49	Local polymer dynamics under strong connectivity constraints: The dendrimer case. Journal of Chemical Physics, 2006, 125, 184907.	1.2	14
50	Static and Dynamic Behavior in Model Dendrimer Melts:Â Toward the Glass Transition. Macromolecules, 2005, 38, 4472-4483.	2.2	41
51	Local Dynamics of Polyethylene and Its Oligomers:Â A Molecular Dynamics Interpretation of the Incoherent Dynamic Structure Factor. Macromolecules, 2003, 36, 8864-8875.	2.2	12
52	Methyl Dynamics and Î²-Relaxation in Polyisobutylene:Â Comparison between Experiment and Molecular Dynamics Simulations. Macromolecules, 2002, 35, 1451-1462.	2.2	25
53	Segmental Dynamics of Atactic Polypropylene As Revealed by Molecular Simulations and Quasielastic Neutron Scattering. Macromolecules, 2002, 35, 7110-7124.	2.2	35
54	Statics and dynamics of model dendrimers as studied by molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 5310-5318.	1.2	127

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55	Local Dynamics of Polyisobutylene Revisited. Macromolecules, 2001, 34, 7232-7235.	2.2	23
56	Short length-scale dynamics of polyisobutylene by molecular dynamics simulations. Physica B: Condensed Matter, 2001, 301, 119-125.	1.3	14
57	An investigation into the local segmental dynamics of polyethylene: An isothermal/isobaric molecular dynamics study. Journal of Chemical Physics, 2001, 115, 2359-2368.	1.2	12
58	Slow modes in local polymer dynamics. Journal of Chemical Physics, 2000, 112, 8225-8228.	1.2	11
59	Nanoscopic-Confinement Effects on Local Dynamics. Physical Review Letters, 2000, 84, 915-918.	2.9	286
60	Effects of density on the local dynamics and conformational statistics of polyethylene: A molecular dynamics study. Journal of Chemical Physics, 2000, 112, 8695-8706.	1.2	19
61	On the Loops-to-Bridges Ratio in Ordered Triblock Copolymers:Â An Investigation by Dielectric Relaxation Spectroscopy and Computer Simulations. Macromolecules, 2000, 33, 523-541.	2.2	74
62	Segmental dynamics of miscible polymer blends: Comparison of the predictions of a concentration fluctuation model to experiment. Journal of Chemical Physics, 1999, 111, 6121-6128.	1.2	105
63	Depolarized light scattering from critical polymer blends. Macromolecular Theory and Simulations, 1999, 8, 179-190.	0.6	2
64	Segmental dynamics and incompatibility in hard/soft polymer blends. Journal of Chemical Physics, 1998, 108, 5997-6005.	1.2	12
65	Confinement Effects on The Local Motion in Nanocomposites. Materials Research Society Symposia Proceedings, 1998, 543, 125.	0.1	0
66	Ordering and viscoelastic relaxation in multiarm star polymer melts. Europhysics Letters, 1997, 39, 617-622.	0.7	65
67	Computer Simulation of Static and Dynamic Behavior of Diblock Copolymer Melts. Macromolecules, 1997, 30, 8463-8472.	2.2	60
68	Photon Correlation Spectroscopy of Interactive Polymer Systems. , 1997, , 131-140.		1
69	Composition Fluctuation Effects on Dielectric Normal-Mode Relaxation in Diblock Copolymers. 2. Disordered State in Proximity to the ODT and Ordered State. Macromolecules, 1996, 29, 1326-1336.	2.2	44
70	Composition Fluctuation Effects on Dielectric Normal-Mode Relaxation in Diblock Copolymers. 1. Weak Segregation Regime. Macromolecules, 1994, 27, 3543-3552.	2.2	48
71	Local and global chain dynamics in diblock copolymer melts. Physica Scripta, 1993, T49A, 237-241.	1.2	8