Vagelis A Harmandaris

List of Publications by Year
in descending order

94 papers	4,665 citations	117453 34 h-index	98622 67 g-index
98 all docs	98 docs citations	98 times ranked	3640 citing authors

#	Article	IF	Citations
1	Aggregation and vesiculation of membrane proteins by curvature-mediated interactions. Nature, 2007, 447, 461-464.	13.7	690
2	Hierarchical Modeling of Polystyrene: From Atomistic to Coarse-Grained Simulations. Macromolecules, 2006, 39, 6708-6719.	2.2	314
3	Crossover from the Rouse to the Entangled Polymer Melt Regime:Â Signals from Long, Detailed Atomistic Molecular Dynamics Simulations, Supported by Rheological Experiments. Macromolecules, 2003, 36, 1376-1387.	2.2	198
4	Dynamics of Polystyrene Melts through Hierarchical Multiscale Simulations. Macromolecules, 2009, 42, 791-802.	2.2	190
5	Detailed Atomistic Simulation of a Polymer Melt/Solid Interface:Â Structure, Density, and Conformation of a Thin Film of Polyethylene Melt Adsorbed on Graphite. Macromolecules, 2005, 38, 5780-5795.	2.2	185
6	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. Macromolecules, 1998, 31, 7934-7943.	2.2	182
7	Multiscale modeling of soft matter: scaling of dynamics. Physical Chemistry Chemical Physics, 2011, 13, 10412.	1.3	163
8	Molecular Dynamics Simulation of a Polymer Melt/Solid Interface:Â Local Dynamics and Chain Mobility in a Thin Film of Polyethylene Melt Adsorbed on Graphite. Macromolecules, 2005, 38, 5796-5809.	2.2	162
9	Comparison Between Coarseâ€Graining Models for Polymer Systems: Two Mapping Schemes for Polystyrene. Macromolecular Chemistry and Physics, 2007, 208, 2109-2120.	1.1	158
10	Coarse-Grained Polymer Melts Based on Isolated Atomistic Chains: Simulation of Polystyrene of Different Tacticities. Macromolecules, 2009, 42, 7579-7588.	2.2	148
11	A novel method for measuring the bending rigidity of model lipid membranes by simulating tethers. Journal of Chemical Physics, 2006, 125, 204905.	1.2	116
12	Dynamics of various polymerâ€“graphene interfacial systems through atomistic molecular dynamics simulations. Soft Matter, 2014, 10, 2876.	1.2	116
13	Effect of Solvent on the Self-Assembly of Dialanine and Diphenylalanine Peptides. Journal of Physical Chemistry B, 2013, 117, 3962-3975.	1.2	94
14	Detailed molecular dynamics simulation of the self-diffusion of n-alkane and cis-1,4 polyisoprene oligomer melts. Journal of Chemical Physics, 2002, 116, 436.	1.2	85
15	Predicting polymer dynamics at multiple length and time scales. Soft Matter, 2009, 5, 3920.	1.2	81
16	Structural and Dynamical Properties of Polyethylene/Graphene Nanocomposites through Molecular Dynamics Simulations. Polymers, 2015, 7, 390-417.	2.0	81
17	Structure Of Biomolecules Through Molecular Dynamics Simulations. Procedia Computer Science, 2019, 156, 69-78.	1.2	76
18	Ethylbenzene Diffusion in Polystyrene:â€‰ United Atom Atomistic/Coarse Grained Simulations and Experiments. Macromolecules, 2007, 40, 7026-7035.	2.2	64

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19	Structure and dynamics of poly(methyl methacrylate)/graphene systems through atomistic molecular dynamics simulations. Journal of Nanoparticle Research, 2013, 15, 1.	0.8	64
20	Fluorescence Correlation Spectroscopy Study of Molecular Probe Diffusion in Polymer Melts. Macromolecules, 2009, 42, 4858-4866.	2.2	61
21	Hierarchical simulations of hybrid polymerâ€“solid materials. Soft Matter, 2013, 9, 6696.	1.2	61
22	Temperature and Pressure Dependence of Polystyrene Dynamics through Molecular Dynamics Simulations and Experiments. Macromolecules, 2011, 44, 393-402.	2.2	60
23	Hierarchical Multiscale Modeling of Polymerâ€“Solid Interfaces: Atomistic to Coarse-Grained Description and Structural and Conformational Properties of Polystyreneâ€“Gold Systems. Macromolecules, 2013, 46, 5741-5750.	2.2	50
24	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. Macromolecules, 2000, 33, 8062-8076.	2.2	49
25	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. Journal of Chemical Physics, 2002, 116, 7656-7665.	1.2	49
26	Atomistic Simulation of Alkanethiol Self-Assembled Monolayers on Different Metal Surfaces via a Quantum, First-Principles Parametrization of the Sulfurâ^Metal Interaction. Journal of Physical Chemistry C, 2007, 111, 6380-6391.	1.5	49
27	Edge-Functionalized Graphene as a Nanofiller: Molecular Dynamics Simulation Study. Macromolecules, 2015, 48, 9024-9038.	2.2	49
28	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. Macromolecules, 2005, 38, 7134-7149.	2.2	48
29	Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene. Journal of Chemical Physics, 2006, 124, 084906.	1.2	44
30	Backmapping coarse-grained macromolecules: An efficient and versatile machine learning approach. Journal of Chemical Physics, 2020, 153, 041101.	1.2	42
31	Dynamics and Rheology of Polymer Melts via Hierarchical Atomistic, Coarse-Grained, and Slip-Spring Simulations. Macromolecules, 2021, 54, 2740-2762.	2.2	40
32	Structural Properties of Atactic Polystyrene of Different Thermal History Obtained from a Multiscale Simulation. Macromolecules, 2009, 42, 384-391.	2.2	38
33	Quantitative Analysis on the Validity of a Coarse-Grained Model for Nonequilibrium Polymeric Liquids under Flow. Macromolecules, 2010, 43, 3156-3160.	2.2	35
34	Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution. Soft Matter, 2019, 15, 289-302.	1.2	35
35	Properties of Benzene Confined between Two Au(111) Surfaces Using a Combined Density Functional Theory and Classical Molecular Dynamics Approach. Journal of Physical Chemistry C, 2011, 115, 14707-14717.	1.5	33
36	Properties of short polystyrene chains confined between two gold surfaces through a combined density functional theory and classical molecular dynamics approach. Soft Matter, 2012, 8, 6320.	1.2	33

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37	The geometry of generalized force matching and related information metrics in coarse-graining of molecular systems. Journal of Chemical Physics, 2015, 143, 084105.	1.2	32
38	Structural and Dynamical Properties of Polystyrene Thin Films Supported by Multiple Graphene Layers. Macromolecules, 2015, 48, 2761-2772.	2.2	32
39	Path-space variational inference for non-equilibrium coarse-grained systems. Journal of Computational Physics, 2016, 314, 355-383.	1.9	32
40	Structural and Conformational Properties of Poly(ethylene oxide)/Silica Nanocomposites: Effect of Confinement. Macromolecules, 2017, 50, 6273-6284.	2.2	32
41	Dynamic Heterogeneity in Fully Miscible Blends of Polystyrene with Oligostyrene. Physical Review Letters, 2013, 110, 165701.	2.9	31
42	Structure, Dynamics, and Apparent Glass Transition of Stereoregular Poly(methyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 542 Td (methac	2.2	31
43	Conformations and Dynamics of Polymer Chains in Cis and Trans Polybutadiene/Silica Nanocomposites through Atomistic Simulations: From the Unentangled to the Entangled Regime. Macromolecules, 2020, 53, 6173-6189.	2.2	30
44	Coarse-graining of polyisoprene melts using inverse Monte Carlo and local density potentials. Journal of Chemical Physics, 2020, 152, 124902.	1.2	27
45	Temperature and Pressure Effects on Local Structure and Chain Packing incis-1,4-Polybutadiene from Detailed Molecular Dynamics Simulations. Macromolecular Theory and Simulations, 2006, 15, 381-393.	0.6	25
46	Structure and Conformation of Stereoregular Poly(methyl methacrylate) Chains Adsorbed on Graphene Oxide and Reduced Graphene Oxide via Atomistic Simulations. Macromolecules, 2019, 52, 3825-3838.	2.2	24
47	A Molecular Dynamics Study of Polymer/<scp>G</scp>raphene Nanocomposites. Macromolecular Symposia, 2013, 331-332, 43-49.	0.4	22
48	Molecular dynamics of polyisoprene/polystyrene oligomer blends: The role of self-concentration and fluctuations on blend dynamics. Journal of Chemical Physics, 2013, 139, 034904.	1.2	22
49	Interphase of a Polymer at a Solid Interface. Macromolecules, 2014, 47, 8459-8465.	2.2	22
50	Dynamics and Structure of Monolayer Polymer Crystallites on Graphene. Nano Letters, 2016, 16, 6994-7000.	4.5	21
51	Structure and dynamics of stereo-regular poly(methyl-methacrylate) melts through atomistic molecular dynamics simulations. Soft Matter, 2018, 14, 1449-1464.	1.2	21
52	Molecular dynamics simulation of temperature and pressure effects on the intermediate length scale dynamics and zero shear rate viscosity of cis-1,4-polybutadiene: Rouse mode analysis and dynamic structure factor spectra. Journal of Non-Newtonian Fluid Mechanics, 2008, 152, 184-194.	1.0	19
53	Interface and Interphase in Polymer Nanocomposites with Bare and Core-Shell Gold Nanoparticles. Polymers, 2021, 13, 541.	2.0	18
54	Equilibration and Deformation of Amorphous Polystyrene: Scaleâ€jumping Simulational Approach. Macromolecular Theory and Simulations, 2008, 17, 290-300.	0.6	17

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55	Parameterization of Coarse-Grained Molecular Interactions through Potential of Mean Force Calculations and Cluster Expansion Techniques. Entropy, 2017, 19, 395.	1.1	17
56	Molecular Simulation Via Connectivityâ€altering Monte Carlo and Scaleâ€jumping Methods: Application to Amorphous Polystyrene. Macromolecular Theory and Simulations, 2008, 17, 393-402.	0.6	15
57	Parametrizing coarse grained models for molecular systems at equilibrium. European Physical Journal: Special Topics, 2016, 225, 1347-1372.	1.2	15
58	Effect of macromolecular architecture on the self-assembly behavior of copolymers in a selective polymer host. Soft Matter, 2018, 14, 9562-9570.	1.2	15
59	Tailoring Interfacial Properties in Polymerâ€“Silica Nanocomposites via Surface Modification: An Atomistic Simulation Study. ACS Applied Polymer Materials, 2021, 3, 2576-2587.	2.0	14
60	Dynamics of Long Entangled Polyisoprene MeltsviaMultiscale Modeling. Macromolecules, 2021, 54, 8693-8713.	2.2	14
61	Quantitative study of equilibrium and non-equilibrium polymer dynamics through systematic hierarchical coarse-graining simulations. Korea Australia Rheology Journal, 2014, 26, 15-28.	0.7	13
62	Parametric sensitivity analysis for stochastic molecular systems using information theoretic metrics. Journal of Chemical Physics, 2015, 143, 014116.	1.2	13
63	Nanostructuring Single-Molecule Polymeric Nanoparticles via Macromolecular Architecture. ACS Nano, 2019, 13, 2439-2449.	7.3	13
64	Investigation of the properties of nanographene in polymer nanocomposites through molecular simulations: dynamics and anisotropic Brownian motion. Physical Chemistry Chemical Physics, 2019, 21, 23843-23854.	1.3	12
65	Mechanical properties of glassy polymer nanocomposites via atomistic and continuum models: The role of interphases. Computer Methods in Applied Mechanics and Engineering, 2022, 395, 114905.	3.4	12
66	Bound Layer Polymer Behavior on Graphene and Graphene Oxide Nanosheets. Macromolecules, 2020, 53, 6190-6203.	2.2	10
67	Coupling between Polymer Conformations and Dynamics Near Amorphous Silica Surfaces: A Direct Insight from Atomistic Simulations. Nanomaterials, 2021, 11, 2075.	1.9	10
68	Self-assembly of Alanine-Isoleucine and Isoleucine-Isoleucine Dipeptides through Atomistic Simulations and Experiments. Journal of Physical Chemistry B, 2020, 124, 7102-7114.	1.2	9
69	Properties of nanographene in polymer nanocomposites through all-atom simulations: Shape fluctuations and rippling. Computational Materials Science, 2020, 172, 109330.	1.4	8
70	Structure and Thermal Stability of wtRop and RM6 Proteins through All-Atom Molecular Dynamics Simulations and Experiments. International Journal of Molecular Sciences, 2021, 22, 5931.	1.8	7
71	Spatio-temporal heterogeneities in nanosegregated single-molecule polymeric nanoparticles. Soft Matter, 2020, 16, 4584-4590.	1.2	6
72	Size and Shape Characteristics of Polystyrene and Poly(ethylene oxide) Star Polymer Melts Studied By Atomistic Simulations. Macromolecular Theory and Simulations, 2021, 30, 2000067.	0.6	6

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73	Gradient of Segmental Dynamics in Stereoregular Poly(methyl methacrylate) Melts Confined between Pristine or Oxidized Graphene Sheets. Polymers, 2021, 13, 830.	2.0	6
74	Polybutadiene Copolymers via Atomistic and Systematic Coarse-Grained Simulations. Macromolecules, 2022, 55, 224-240.	2.2	5
75	Atomistic Molecular Dynamics Simulations of Polymer/Graphene Nanostructured Systems. Materials Today: Proceedings, 2018, 5, 27472-27481.	0.9	4
76	Modelling of novel polymer materials through atomistic molecular dynamics simulations. Procedia Computer Science, 2018, 136, 341-350.	1.2	4
77	Dynamical heterogeneities in non-entangled polystyrene and poly(ethylene oxide) star melts. Physics of Fluids, 2020, 32, 127117.	1.6	4
78	Self-assembly of diphenylalanine peptides on graphene via detailed atomistic simulations. Physical Chemistry Chemical Physics, 2020, 22, 27645-27657.	1.3	3
79	From Order to Disorder of Alkanethiol Self-Assembled Monolayers on Complex Au (211), (221), and (311) Surfaces: Impact of the Substrate. Journal of Physical Chemistry C, 2021, 125, 3495-3508.	1.5	3
80	How Does the Number of Arms Affect the Properties of Mikto-Arm Stars in a Selective Oligomeric Matrix? Insights from Atomistic Simulations. ACS Omega, 2021, 6, 1138-1148.	1.6	3
81	Bio-waste to Bio-plastic (B2B): Production of Compostable Bio-Plastics from Food Waste. Proceedings (mdpi), 2019, 30, 47.	0.2	3
82	Path space force matching and relative entropy methods for coarse-graining molecular systems at transient regimes. Procedia Computer Science, 2018, 136, 331-340.	1.2	2
83	Study of the transient dynamics of coarse-grained molecular systems with the path-space force-matching method. Procedia Computer Science, 2019, 156, 59-68.	1.2	2
84	Data-driven uncertainty quantification for systematic coarse-grained models. Soft Materials, 2020, 18, 348-368.	0.8	2
85	Modeling the evolution of COVID-19 via compartmental and particle-based approaches: Application to the Cyprus case. PLoS ONE, 2021, 16, e0250709.	1.1	2
86	Artificial Intelligence as the Driver of Computational Science: preface to YSCâ€™2020. Procedia Computer Science, 2020, 178, 1-7.	1.2	2
87	Wall-Spring Thermostat: A Novel Approach for Controlling the Dynamics of Soft Coarse-Grained Polymer Fluids at Surfaces. Macromolecules, 2022, 55, 5550-5566.	2.2	2
88	Mikto-Arm Stars as Soft-Patchy Particles: From Building Blocks to Mesoscopic Structures. Polymers, 2021, 13, 1114.	2.0	1
89	Molecular Dynamics Simulations of Polymers. , 2004, , .		1
90	FROM ATOMISTIC TO SYSTEMATIC COARSE-GRAINED MODELS FOR MOLECULAR SYSTEMS. , 2017, , .		1

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91	Neural Network Potential Surfaces: A Comparison of two Approaches. Procedia Computer Science, 2020, 178, 345-354.	1.2	1
92	A molecular dynamics study of polymer/graphene interfacial systems. , 2014, , .		0
93	Atomistic simulation of graphene-based polymer nanocomposites. AIP Conference Proceedings, 2016, , .	0.3	0
94	Systematic Coarse-Grained Models for Molecular Systems Using Entropy. Proceedings (mdpi), 2020, 46, 27.	0.2	0