Vagelis A Harmandaris

List of Publications by Year in Descending Order

87 papers	3,910 citations	31 h-index	62 g-index
98 ext. papers	4,302 ext. citations	4.6 avg, IF	5.66 L-index

#	Paper	IF	Citations
87	Polybutadiene Copolymers via Atomistic and Systematic Coarse-Grained Simulations. *Macromolecules*, **2022**, 55, 224-240	5.5	1
86	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	5.7	2
85	Tailoring Interfacial Properties in Polymer–Silica Nanocomposites via Surface Modification: An Atomistic Simulation Study. *ACS Applied Polymer Materials*, **2021**, 3, 2576-2587	4.3	4
84	Modeling the evolution of COVID-19 via compartmental and particle-based approaches: Application to the Cyprus case. *PLoS ONE*, **2021**, 16, e0250709	3.7	2
83	Size and Shape Characteristics of Polystyrene and Poly(ethylene oxide) Star Polymer Melts Studied By Atomistic Simulations. *Macromolecular Theory and Simulations*, **2021**, 30, 2000067	1.5	1
82	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	3.8	0
81	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	3.9	1
80	Dynamics and Rheology of Polymer Melts via Hierarchical Atomistic, Coarse-Grained, and Slip-Spring Simulations. *Macromolecules*, **2021**, 54, 2740-2762	5.5	12
79	Interface and Interphase in Polymer Nanocomposites with Bare and Core-Shell Gold Nanoparticles. *Polymers*, **2021**, 13,	4.5	5
78	Gradient of Segmental Dynamics in Stereoregular Poly(Methyl Methacrylate) Melts Confined between Pristine or Oxidized Graphene Sheets. *Polymers*, **2021**, 13,	4.5	3
77	Coupling between Polymer Conformations and Dynamics Near Amorphous Silica Surfaces: A Direct Insight from Atomistic Simulations. *Nanomaterials*, **2021**, 11,	5.4	2
76	Dynamics of Long Entangled Polyisoprene Melts via Multiscale Modeling. *Macromolecules*, **2021**, 54, 8693-8713	5.5	2
75	Self-assembly of diphenylalanine peptides on graphene detailed atomistic simulations. *Physical Chemistry Chemical Physics*, **2020**, 22, 27645-27657	3.6	3
74	Coarse-graining of polyisoprene melts using inverse Monte Carlo and local density potentials. *Journal of Chemical Physics*, **2020**, 152, 124902	3.9	14
73	Spatio-temporal heterogeneities in nanosegregated single-molecule polymeric nanoparticles. *Soft Matter*, **2020**, 16, 4584-4590	3.6	4
72	Systematic Coarse-Grained Models for Molecular Systems Using Entropy. *Proceedings (mdpi)*, **2020**, 46, 27	0.3	
71	Neural Network Potential Surfaces: A Comparison of two Approaches. *Procedia Computer Science*, **2020**, 178, 345-354	1.6	1

70	Artificial Intelligence as the Driver of Computational Science: preface to YSC2020. *Procedia Computer Science*, **2020**, 178, 1-7	1.6	0
69	Dynamical heterogeneities in non-entangled polystyrene and poly(ethylene oxide) star melts. *Physics of Fluids*, **2020**, 32, 127117	4.4	1
68	Properties of nanographene in polymer nanocomposites through all-atom simulations: Shape fluctuations and rippling. *Computational Materials Science*, **2020**, 172, 109330	3.2	8
67	Self-assembly of Alanine-Isoleucine and Isoleucine-Isoleucine Dipeptides through Atomistic Simulations and Experiments. *Journal of Physical Chemistry B*, **2020**, 124, 7102-7114	3.4	3
66	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	5.5	17
65	Data-driven uncertainty quantification for systematic coarse-grained models. *Soft Materials*, **2020**, 18, 348-368	1.7	1
64	Bound Layer Polymer Behavior on Graphene and Graphene Oxide Nanosheets. *Macromolecules*, **2020**, 53, 6190-6203	5.5	6
63	Backmapping coarse-grained macromolecules: An efficient and versatile machine learning approach. *Journal of Chemical Physics*, **2020**, 153, 041101	3.9	19
62	Study of the transient dynamics of coarse-grained molecular systems with the path-space force-matching method. *Procedia Computer Science*, **2019**, 156, 59-68	1.6	1
61	Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution. *Soft Matter*, **2019**, 15, 289-302	3.6	23
60	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	5.5	21
59	Nanostructuring Single-Molecule Polymeric Nanoparticles via Macromolecular Architecture. *ACS Nano*, **2019**, 13, 2439-2449	16.7	10
58	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	3.6	7
57	Structure Of Biomolecules Through Molecular Dynamics Simulations. *Procedia Computer Science*, **2019**, 156, 69-78	1.6	31
56	Bio-waste to Bio-plastic (B2B): Production of Compostable Bio-Plastics from Food Waste. *Proceedings (mdpi)*, **2019**, 30, 47	0.3	3
55	Structure and dynamics of stereo-regular poly(methyl-methacrylate) melts through atomistic molecular dynamics simulations. *Soft Matter*, **2018**, 14, 1449-1464	3.6	14
54	Atomistic Molecular Dynamics Simulations of Polymer/Graphene Nanostructured Systems. *Materials Today: Proceedings*, **2018**, 5, 27472-27481	1.4	0
53	Modelling of novel polymer materials through atomistic molecular dynamics simulations. *Procedia Computer Science*, **2018**, 136, 341-350	1.6	3

52	Path space force matching and relative entropy methods for coarse-graining molecular systems at transient regimes. *Procedia Computer Science*, **2018**, 136, 331-340	1.6	1
51	Effect of macromolecular architecture on the self-assembly behavior of copolymers in a selective polymer host. *Soft Matter*, **2018**, 14, 9562-9570	3.6	12
50	Structure, Dynamics, and Apparent Glass Transition of Stereoregular Poly(methyl methacrylate)/Graphene Interfaces through Atomistic Simulations. *Macromolecules*, **2018**, 51, 7518-7532	5.5	26
49	Structural and Conformational Properties of Poly(ethylene oxide)/Silica Nanocomposites: Effect of Confinement. *Macromolecules*, **2017**, 50, 6273-6284	5.5	27
48	Parameterization of Coarse-Grained Molecular Interactions through Potential of Mean Force Calculations and Cluster Expansion Techniques. *Entropy*, **2017**, 19, 395	2.8	14
47	Dynamics and Structure of Monolayer Polymer Crystallites on Graphene. *Nano Letters*, **2016**, 16, 6994-7000	12.5	19
46	Parametrizing coarse grained models for molecular systems at equilibrium. *European Physical Journal: Special Topics*, **2016**, 225, 1347-1372	2.3	11
45	Path-space variational inference for non-equilibrium coarse-grained systems. *Journal of Computational Physics*, **2016**, 314, 355-383	4.1	26
44	Structural and Dynamical Properties of Polystyrene Thin Films Supported by Multiple Graphene Layers. *Macromolecules*, **2015**, 48, 2761-2772	5.5	29
43	Parametric sensitivity analysis for stochastic molecular systems using information theoretic metrics. *Journal of Chemical Physics*, **2015**, 143, 014116	3.9	13
42	The geometry of generalized force matching and related information metrics in coarse-graining of molecular systems. *Journal of Chemical Physics*, **2015**, 143, 084105	3.9	21
41	Structural and Dynamical Properties of Polyethylene/Graphene Nanocomposites through Molecular Dynamics Simulations. *Polymers*, **2015**, 7, 390-417	4.5	71
40	Edge-Functionalized Graphene as a Nanofiller: Molecular Dynamics Simulation Study. *Macromolecules*, **2015**, 48, 9024-9038	5.5	45
39	Dynamics of various polymer-graphene interfacial systems through atomistic molecular dynamics simulations. *Soft Matter*, **2014**, 10, 2876-88	3.6	98
38	Interphase of a Polymer at a Solid Interface. *Macromolecules*, **2014**, 47, 8459-8465	5.5	19
37	Quantitative study of equilibrium and non-equilibrium polymer dynamics through systematic hierarchical coarse-graining simulations **2014**, 26, 15-28		11
36	Structure and dynamics of poly(methyl methacrylate)/graphene systems through atomistic molecular dynamics simulations. *Journal of Nanoparticle Research*, **2013**, 15, 1	2.3	57
35	A Molecular Dynamics Study of Polymer/Graphene Nanocomposites. *Macromolecular Symposia*, **2013**, 331-332, 43-49	0.8	21

34	Hierarchical Multiscale Modeling of Polymer–Solid Interfaces: Atomistic to Coarse-Grained Description and Structural and Conformational Properties of Polystyrene–Gold Systems. *Macromolecules*, **2013**, 46, 5741-5750	5.5	41
33	Effect of solvent on the self-assembly of dialanine and diphenylalanine peptides. *Journal of Physical Chemistry B*, **2013**, 117, 3962-75	3.4	73
32	Hierarchical simulations of hybrid polymer–solid materials. *Soft Matter*, **2013**, 9, 6696	3.6	56
31	Molecular dynamics of polyisoprene/polystyrene oligomer blends: the role of self-concentration and fluctuations on blend dynamics. *Journal of Chemical Physics*, **2013**, 139, 034904	3.9	20
30	Dynamic heterogeneity in fully miscible blends of polystyrene with oligostyrene. *Physical Review Letters*, **2013**, 110, 165701	7.4	29
29	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	3.6	31
28	Multiscale modeling of soft matter: scaling of dynamics. *Physical Chemistry Chemical Physics*, **2011**, 13, 10412-20	3.6	133
27	Temperature and Pressure Dependence of Polystyrene Dynamics through Molecular Dynamics Simulations and Experiments. *Macromolecules*, **2011**, 44, 393-402	5.5	53
26	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	3.8	31
25	Quantitative Analysis on the Validity of a Coarse-Grained Model for Nonequilibrium Polymeric Liquids under Flow. *Macromolecules*, **2010**, 43, 3156-3160	5.5	32
24	Dynamics of Polystyrene Melts through Hierarchical Multiscale Simulations. *Macromolecules*, **2009**, 42, 791-802	5.5	168
23	Fluorescence Correlation Spectroscopy Study of Molecular Probe Diffusion in Polymer Melts. *Macromolecules*, **2009**, 42, 4858-4866	5.5	54
22	Coarse-Grained Polymer Melts Based on Isolated Atomistic Chains: Simulation of Polystyrene of Different Tacticities. *Macromolecules*, **2009**, 42, 7579-7588	5.5	134
21	Structural Properties of Atactic Polystyrene of Different Thermal History Obtained from a Multiscale Simulation. *Macromolecules*, **2009**, 42, 384-391	5.5	36
20	Predicting polymer dynamics at multiple length and time scales. *Soft Matter*, **2009**, 5, 3920	3.6	70
19	Equilibration and Deformation of Amorphous Polystyrene: Scale-jumping Simulational Approach. *Macromolecular Theory and Simulations*, **2008**, 17, 290-300	1.5	17
18	Molecular Simulation Via Connectivity-altering Monte Carlo and Scale-jumping Methods: Application to Amorphous Polystyrene. *Macromolecular Theory and Simulations*, **2008**, 17, 393-402	1.5	13
17	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	2.7	14

16	Ethylbenzene Diffusion in Polystyrene: United Atom Atomistic/Coarse Grained Simulations and Experiments. *Macromolecules*, **2007**, 40, 7026-7035	5.5	60
15	Atomistic Simulation of Alkanethiol Self-Assembled Monolayers on Different Metal Surfaces via a Quantum, First-Principles Parametrization of the Sulfur Metal Interaction. *Journal of Physical Chemistry C*, **2007**, 111, 6380-6391	3.8	46
14	Comparison Between Coarse-Graining Models for Polymer Systems: Two Mapping Schemes for Polystyrene. *Macromolecular Chemistry and Physics*, **2007**, 208, 2109-2120	2.6	142
13	Aggregation and vesiculation of membrane proteins by curvature-mediated interactions. *Nature*, **2007**, 447, 461-4	50.4	595
12	Temperature and Pressure Effects on Local Structure and Chain Packing in cis-1,4-Polybutadiene from Detailed Molecular Dynamics Simulations. *Macromolecular Theory and Simulations*, **2006**, 15, 381-393	1.5	20
11	A novel method for measuring the bending rigidity of model lipid membranes by simulating tethers. *Journal of Chemical Physics*, **2006**, 125, 204905	3.9	101
10	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	3.9	33
9	Hierarchical Modeling of Polystyrene: From Atomistic to Coarse-Grained Simulations. *Macromolecules*, **2006**, 39, 6708-6719	5.5	288
8	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
7	Molecular Dynamics Simulation of a Polymer Melt/Solid Interface: Local Dynamics and Chain Mobility in a Thin Film of Polyethylene Melt Adsorbed on Graphite. *Macromolecules*, **2005**, 38, 5796-5809	5.5	152
6	Detailed Atomistic Simulation of a Polymer Melt/Solid Interface: Structure, Density, and Conformation of a Thin Film of Polyethylene Melt Adsorbed on Graphite. *Macromolecules*, **2005**, 38, 5780-5795	5.5	166
5	Crossover from the Rouse to the Entangled Polymer Melt Regime: Signals from Long, Detailed Atomistic Molecular Dynamics Simulations, Supported by Rheological Experiments. *Macromolecules* , **2003**, 36, 1376-1387	5.5	179
4	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. *Journal of Chemical Physics*, **2002**, 116, 7656-7665	3.9	46
3	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	3.9	78
2	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. *Macromolecules*, **2000**, 33, 8062-8076	5.5	41
1	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. *Macromolecules*, **1998**, 31, 7934-7943	5.5	159