Kostas Ch Daoulas

List of Publications by Year
in descending order

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Version: 2024-02-01

57 papers	2,821 citations	201658 27 h-index	168376 53 g-index
57 all docs	57 docs citations	57 times ranked	2269 citing authors

#	Article	IF	Citations
1	Directed Self-Assembly of Block Copolymers for Nanolithography: Fabrication of Isolated Features and Essential Integrated Circuit Geometries. ACS Nano, 2007, 1, 168-175.	14.6	424
2	Single chain in mean field simulations: Quasi-instantaneous field approximation and quantitative comparison with Monte Carlo simulations. Journal of Chemical Physics, 2006, 125, 184904.	3.0	211
3	Monte Carlo Simulations of a Coarse Grain Model for Block Copolymers and Nanocomposites. Macromolecules, 2008, 41, 4989-5001.	4.8	198
4	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.	4.8	185
5	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.	4.8	162
6	Morphology of multi-component polymer systems: single chain in mean field simulation studies. Soft Matter, 2006, 2, 573-583.	2.7	134
7	Hierarchical Assembly of Nanoparticle Superstructures from Block Copolymer-Nanoparticle Composites. Physical Review Letters, 2008, 100, 148303.	7.8	126
8	Fabrication of Complex Three-Dimensional Nanostructures from Self-Assembling Block Copolymer Materials on Two-Dimensional Chemically Patterned Templates with Mismatched Symmetry. Physical Review Letters, 2006, 96, 036104.	7.8	110
9	Calculating the free energy of self-assembled structures by thermodynamic integration. Journal of Chemical Physics, 2008, 128, 024903.	3.0	87
10	Remediation of Line Edge Roughness in Chemical Nanopatterns by the Directed Assembly of Overlying Block Copolymer Films. Macromolecules, 2010, 43, 2334-2342.	4.8	81
11	Directed Copolymer Assembly on Chemical Substrate Patterns:â€‰ A Phenomenological and Single-Chain-in-Mean-Field Simulations Study of the Influence of Roughness in the Substrate Pattern. Langmuir, 2008, 24, 1284-1295.	3.5	70
12	Single-chain dynamics in a homogeneous melt and a lamellar microphase: A comparison between Smart Monte Carlo dynamics, slithering-snake dynamics, and slip-link dynamics. Journal of Chemical Physics, 2008, 129, 164906.	3.0	67
13	Equilibration of High Molecular Weight Polymer Melts: A Hierarchical Strategy. ACS Macro Letters, 2014, 3, 198-203.	4.8	67
14	Morphology and Charge Transport in P3HT: A Theoristâ€™s Perspective. Advances in Polymer Science, 2014, , 139-180.	0.8	61
15	Nematic Ordering, Conjugation, and Density of States of Soluble Polymeric Semiconductors. Macromolecules, 2013, 46, 5762-5774.	4.8	56
16	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. Macromolecules, 2005, 38, 7134-7149.	4.8	48
17	Detailed atomistic Monte Carlo simulation of grafted polymer melts. I. Thermodynamic and conformational properties. Journal of Chemical Physics, 2002, 116, 11028-11038.	3.0	40
18	Polymerâ€“solid contacts described by soft, coarse-grained models. Physical Chemistry Chemical Physics, 2011, 13, 10491.	2.8	38

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19	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. Macromolecules, 2004, 37, 5093-5109.	4.8	37
20	Generic Model for Lamellar Self-Assembly in Conjugated Polymers: Linking Mesoscopic Morphology and Charge Transport in P3HT. Macromolecules, 2019, 52, 968-981.	4.8	36
21	Self-Assembly in Thin Films of Mixtures of Block Copolymers and Homopolymers Interacting by Hydrogen Bonds. Macromolecules, 2010, 43, 7734-7743.	4.8	35
22	Effect of Mesoscale Ordering on the Density of States of Polymeric Semiconductors. Macromolecular Rapid Communications, 2015, 36, 1047-1053.	3.9	35
23	Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution. Soft Matter, 2019, 15, 289-302.	2.7	35
24	Measuring excess free energies of self-assembled membrane structures. Faraday Discussions, 2010, 144, 369-391.	3.2	34
25	Speeding Up Intrinsically Slow Collective Processes in Particle Simulations by Concurrent Coupling to a Continuum Description. Physical Review Letters, 2011, 107, 227801.	7.8	32
26	Computing free energies of interfaces in self-assembling systems. Physical Chemistry Chemical Physics, 2009, 11, 2087.	2.8	30
27	A New Coarse Grained Particleâ€Toâ€Mesh Scheme for Modeling Soft Matter. Macromolecular Chemistry and Physics, 2013, 214, 214-224.	2.2	28
28	Simulations of nematic homopolymer melts using particle-based models with interactions expressed through collective variables. Journal of Physics Condensed Matter, 2012, 24, 284121.	1.8	26
29	Fluctuation spectra in polymer nematics and Frank elastic constants: a coarse-grained modelling study. Soft Matter, 2015, 11, 532-544.	2.7	25
30	Phase behaviour of quasi-block copolymers: A DFT-based Monte-Carlo study. Soft Matter, 2009, 5, 4499.	2.7	23
31	An Efficient Monte Carlo Algorithm for the Fast Equilibration and Atomistic Simulation of Alkanethiol Self-Assembled Monolayers on a Au(111) Substrate. Journal of Physical Chemistry B, 2008, 112, 1198-1211.	2.6	20
32	Directed assembly of copolymer materials on patterned substrates: Balance of simple symmetries in complex structures. Journal of Polymer Science, Part B: Polymer Physics, 2006, 44, 2589-2604.	2.1	19
33	Directed Assembly of Supramolecular Copolymers in Thin Films: Thermodynamic and Kinetic Advantages. Physical Review Letters, 2010, 105, 108301.	7.8	19
34	Quasi-Block Copolymers: Design, Synthesis, and Evidence for Their Formation in Solution and in the Melt. Macromolecules, 2011, 44, 9773-9781.	4.8	18
35	Communication: One size fits all: Equilibrating chemically different polymer liquids through universal long-wavelength description. Journal of Chemical Physics, 2015, 142, 221102.	3.0	18
36	Maier-Saupe model of polymer nematics: Comparing free energies calculated with Self Consistent Field theory and Monte Carlo simulations. Journal of Chemical Physics, 2016, 145, 184901.	3.0	17

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37	Temperature-Dependence of Persistence Length Affects Phenomenological Descriptions of Aligning Interactions in Nematic Semiconducting Polymers. Chemistry of Materials, 2018, 30, 748-761.	6.7	17
38	Ink Formulation for Printed Organic Electronics: Investigating Effects of Aggregation on Structure and Rheology of Functional Inks Based on Conjugated Polymers in Mixed Solvents. Advanced Materials Technologies, 2021, 6, 2000335.	5.8	17
39	Variable Connectivity Methods for the Atomistic Monte Carlo Simulation of Inhomogeneous and/or Anisotropic Polymer Systems of Precisely Defined Chain Length Distribution:Â Tuning the Spectrum of Chain Relative Chemical Potentials. Macromolecules, 2003, 36, 6674-6682.	4.8	15
40	Exploring thermodynamic stability of the stalk fusion-intermediate with three-dimensional self-consistent field theory calculations. Soft Matter, 2013, 9, 4097.	2.7	13
41	The Cassie-Wenzel transition of fluids on nanostructured substrates: Macroscopic force balance versus microscopic density-functional theory. Journal of Chemical Physics, 2016, 145, 134703.	3.0	13
42	Exploring Disordered Morphologies of Blends and Block Copolymers for Light-Emitting Diodes with Mesoscopic Simulations. Macromolecules, 2020, 53, 523-538.	4.8	12
43	Comparison of Simulations of Lipid Membranes with Membranes of Block Copolymers. Advances in Polymer Science, 2009, , 43-85.	0.8	10
44	Equilibrating high-molecular-weight symmetric and miscible polymer blends with hierarchical back-mapping. Journal of Physics Condensed Matter, 2018, 30, 174001.	1.8	10
45	Can Soft Models Describe Polymer Knots?. Macromolecules, 2020, 53, 10475-10486.	4.8	9
46	Thermodynamics of a Compressible Maier-Saupe Model Based on the Self-Consistent Field Theory of Wormlike Polymer. Polymers, 2017, 9, 48.	4.5	8
47	Splayâ€“density coupling in semiflexible main-chain nematic polymers with hairpins. Soft Matter, 2018, 14, 5898-5905.	2.7	8
48	Detailed atomistic Monte Carlo simulation of grafted polymer melts: II. Orientational order and nuclear magnetic resonance spectra. Journal of Chemical Physics, 2003, 118, 1521-1532.	3.0	7
49	Comparing equilibration schemes of high-molecular-weight polymer melts with topological indicators. Journal of Physics Condensed Matter, 2021, 33, 204003.	1.8	7
50	Studying polymer solutions with particle-based models linked to classical density functionals: co-non-solvency. Soft Matter, 2018, 14, 9282-9295.	2.7	6
51	Dynamic coarse-graining of polymer systems using mobility functions. Journal of Physics Condensed Matter, 2021, 33, 194004.	1.8	5
52	Studying PMMA films on silica surfaces with generic microscopic and mesoscale models. European Physical Journal: Special Topics, 2016, 225, 1423-1440.	2.6	4
53	Ordering of Diblock Copolymer Materials on Patterned Substrates: a Single Chain in Mean Field Simulation Study. Macromolecular Symposia, 2007, 252, 68-75.	0.7	2
54	Comparison of Simulations of Lipid Membranes with Membranes of Block Copolymers. Advances in Polymer Science, 2009, , .	0.8	2

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55	Top-Down Hybrid Models of Polymers. , 2020, , 1411-1430.		2
56	Mesoscopic Modeling of a Highly-Ordered Sanidic Polymer Mesophase and Comparison With Experimental Data. Journal of Physical Chemistry B, 2022, 126, 2285-2298.	2.6	2
57	Top-Down Hybrid Models of Polymers. , 2018, , 1-20.		0