Kostas Ch Daoulas

List of Publications by Year
in descending order

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57 papers	2,821 citations	230014 27 h-index	190340 53 g-index
57 all docs	57 docs citations	57 times ranked	2626 citing authors

#	Article	IF	Citations
1	Mesoscopic Modeling of a Highly-Ordered Sanidic Polymer Mesophase and Comparison With Experimental Data. Journal of Physical Chemistry B, 2022, 126, 2285-2298.	1.2	2
2	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.	3.0	17
3	Dynamic coarse-graining of polymer systems using mobility functions. Journal of Physics Condensed Matter, 2021, 33, 194004.	0.7	5
4	Comparing equilibration schemes of high-molecular-weight polymer melts with topological indicators. Journal of Physics Condensed Matter, 2021, 33, 204003.	0.7	7
5	Can Soft Models Describe Polymer Knots?. Macromolecules, 2020, 53, 10475-10486.	2.2	9
6	Exploring Disordered Morphologies of Blends and Block Copolymers for Light-Emitting Diodes with Mesoscopic Simulations. Macromolecules, 2020, 53, 523-538.	2.2	12
7	Top-Down Hybrid Models of Polymers. , 2020, , 1411-1430.		2
8	Generic Model for Lamellar Self-Assembly in Conjugated Polymers: Linking Mesoscopic Morphology and Charge Transport in P3HT. Macromolecules, 2019, 52, 968-981.	2.2	36
9	Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution. Soft Matter, 2019, 15, 289-302.	1.2	35
10	Temperature-Dependence of Persistence Length Affects Phenomenological Descriptions of Aligning Interactions in Nematic Semiconducting Polymers. Chemistry of Materials, 2018, 30, 748-761.	3.2	17
11	Equilibrating high-molecular-weight symmetric and miscible polymer blends with hierarchical back-mapping. Journal of Physics Condensed Matter, 2018, 30, 174001.	0.7	10
12	Studying polymer solutions with particle-based models linked to classical density functionals: co-non-solvency. Soft Matter, 2018, 14, 9282-9295.	1.2	6
13	Top-Down Hybrid Models of Polymers. , 2018, , 1-20.		0
14	Splayâ€“density coupling in semiflexible main-chain nematic polymers with hairpins. Soft Matter, 2018, 14, 5898-5905.	1.2	8
15	Thermodynamics of a Compressible Maier-Saupe Model Based on the Self-Consistent Field Theory of Wormlike Polymer. Polymers, 2017, 9, 48.	2.0	8
16	The Cassie-Wenzel transition of fluids on nanostructured substrates: Macroscopic force balance versus microscopic density-functional theory. Journal of Chemical Physics, 2016, 145, 134703.	1.2	13
17	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.	1.2	17
18	Studying PMMA films on silica surfaces with generic microscopic and mesoscale models. European Physical Journal: Special Topics, 2016, 225, 1423-1440.	1.2	4

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19	Effect of Mesoscale Ordering on the Density of States of Polymeric Semiconductors. Macromolecular Rapid Communications, 2015, 36, 1047-1053.	2.0	35
20	Communication: One size fits all: Equilibrating chemically different polymer liquids through universal long-wavelength description. Journal of Chemical Physics, 2015, 142, 221102.	1.2	18
21	Fluctuation spectra in polymer nematics and Frank elastic constants: a coarse-grained modelling study. Soft Matter, 2015, 11, 532-544.	1.2	25
22	Morphology and Charge Transport in P3HT: A Theoristâ€™s Perspective. Advances in Polymer Science, 2014, , 139-180.	0.4	61
23	Equilibration of High Molecular Weight Polymer Melts: A Hierarchical Strategy. ACS Macro Letters, 2014, 3, 198-203.	2.3	67
24	Nematic Ordering, Conjugation, and Density of States of Soluble Polymeric Semiconductors. Macromolecules, 2013, 46, 5762-5774.	2.2	56
25	A New Coarse Grained Particleâ€Toâ€Mesh Scheme for Modeling Soft Matter. Macromolecular Chemistry and Physics, 2013, 214, 214-224.	1.1	28
26	Exploring thermodynamic stability of the stalk fusion-intermediate with three-dimensional self-consistent field theory calculations. Soft Matter, 2013, 9, 4097.	1.2	13
27	Simulations of nematic homopolymer melts using particle-based models with interactions expressed through collective variables. Journal of Physics Condensed Matter, 2012, 24, 284121.	0.7	26
28	Polymerâ€“solid contacts described by soft, coarse-grained models. Physical Chemistry Chemical Physics, 2011, 13, 10491.	1.3	38
29	Quasi-Block Copolymers: Design, Synthesis, and Evidence for Their Formation in Solution and in the Melt. Macromolecules, 2011, 44, 9773-9781.	2.2	18
30	Speeding Up Intrinsically Slow Collective Processes in Particle Simulations by Concurrent Coupling to a Continuum Description. Physical Review Letters, 2011, 107, 227801.	2.9	32
31	Directed Assembly of Supramolecular Copolymers in Thin Films: Thermodynamic and Kinetic Advantages. Physical Review Letters, 2010, 105, 108301.	2.9	19
32	Remediation of Line Edge Roughness in Chemical Nanopatterns by the Directed Assembly of Overlying Block Copolymer Films. Macromolecules, 2010, 43, 2334-2342.	2.2	81
33	Measuring excess free energies of self-assembled membrane structures. Faraday Discussions, 2010, 144, 369-391.	1.6	34
34	Self-Assembly in Thin Films of Mixtures of Block Copolymers and Homopolymers Interacting by Hydrogen Bonds. Macromolecules, 2010, 43, 7734-7743.	2.2	35
35	Phase behaviour of quasi-block copolymers: A DFT-based Monte-Carlo study. Soft Matter, 2009, 5, 4499.	1.2	23
36	Comparison of Simulations of Lipid Membranes with Membranes of Block Copolymers. Advances in Polymer Science, 2009, , 43-85.	0.4	10

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37	Computing free energies of interfaces in self-assembling systems. Physical Chemistry Chemical Physics, 2009, 11, 2087.	1.3	30
38	Comparison of Simulations of Lipid Membranes with Membranes of Block Copolymers. Advances in Polymer Science, 2009, , .	0.4	2
39	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.	1.6	70
40	Hierarchical Assembly of Nanoparticle Superstructures from Block Copolymer-Nanoparticle Composites. Physical Review Letters, 2008, 100, 148303.	2.9	126
41	Monte Carlo Simulations of a Coarse Grain Model for Block Copolymers and Nanocomposites. Macromolecules, 2008, 41, 4989-5001.	2.2	198
42	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.	1.2	20
43	Calculating the free energy of self-assembled structures by thermodynamic integration. Journal of Chemical Physics, 2008, 128, 024903.	1.2	87
44	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.	1.2	67
45	Ordering of Diblock Copolymer Materials on Patterned Substrates: a Single Chain in Mean Field Simulation Study. Macromolecular Symposia, 2007, 252, 68-75.	0.4	2
46	Directed Self-Assembly of Block Copolymers for Nanolithography: Fabrication of Isolated Features and Essential Integrated Circuit Geometries. ACS Nano, 2007, 1, 168-175.	7.3	424
47	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.	2.9	110
48	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.	2.4	19
49	Morphology of multi-component polymer systems: single chain in mean field simulation studies. Soft Matter, 2006, 2, 573-583.	1.2	134
50	Single chain in mean field simulations: Quasi-instantaneous field approximation and quantitative comparison with Monte Carlo simulations. Journal of Chemical Physics, 2006, 125, 184904.	1.2	211
51	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
52	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
53	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
54	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. Macromolecules, 2004, 37, 5093-5109.	2.2	37

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55	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.	2.2	15
56	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.	1.2	7
57	Detailed atomistic Monte Carlo simulation of grafted polymer melts. I. Thermodynamic and conformational properties. Journal of Chemical Physics, 2002, 116, 11028-11038.	1.2	40