

Kris T Delaney

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

120
papers

5,419
citations

37
h-index

71
g-index

132
ext. papers

6,212
ext. citations

6.3
avg, IF

6
L-index

#	Paper	IF	Citations
120	Direct free energy evaluation of classical and quantum many-body systems via field-theoretic simulation.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022 , 119, e2201804119	11.5	3
119	Self-consistent field theory study of polymer-mediated colloidal interactions in solution: Depletion effects and induced forces. <i>Journal of Chemical Physics</i> , 2021 , 155, 154903	3.9	3
118	Molecularly Informed Field Theories from Bottom-up Coarse-Graining.. <i>ACS Macro Letters</i> , 2021 , 10, 576-583	6.3	5
117	Liquid-liquid phase separation of Tau by self and complex coacervation. <i>Protein Science</i> , 2021 , 30, 1393-1407	14.9	14
116	Electrostatic Manipulation of Phase Behavior in Immiscible Charged Polymer Blends. <i>Macromolecules</i> , 2021 , 54, 2604-2616	5.5	7
115	Open-source platform for block polymer formulation design using particle swarm optimization. <i>European Physical Journal E</i> , 2021 , 44, 115	1.5	1
114	Rapid Generation of Block Copolymer Libraries Using Automated Chromatographic Separation. <i>Journal of the American Chemical Society</i> , 2020 , 142, 9843-9849	16.4	13
113	Effect of an electric field on the stability of binary dielectric fluid mixtures. <i>Journal of Chemical Physics</i> , 2020 , 152, 234901	3.9	5
112	Connecting Solute Diffusion to Morphology in Triblock Copolymer Membranes. <i>Macromolecules</i> , 2020 , 53, 2336-2343	5.5	8
111	The Role of Backbone Polarity on Aggregation and Conduction of Ions in Polymer Electrolytes. <i>Journal of the American Chemical Society</i> , 2020 , 142, 7055-7065	16.4	53
110	Dehydration entropy drives liquid-liquid phase separation by molecular crowding. <i>Communications Chemistry</i> , 2020 , 3,	6.3	43
109	Numerical Simulation of Finite-Temperature Field Theory for Interacting Bosons. <i>Physical Review Letters</i> , 2020 , 124, 070601	7.4	2
108	Extreme Deflection of Phase Boundaries and Chain Bridging in A(BA?)n Miktoarm Star Polymers. <i>Macromolecules</i> , 2020 , 53, 513-522	5.5	23
107	Complete Photonic Band Gaps with Nonfrustrated ABC Bottlebrush Block Polymers. <i>ACS Macro Letters</i> , 2020 , 9, 1074-1080	6.6	13
106	Architecture Effects in Complex Spherical Assemblies of (AB)n-Type Block Copolymers. <i>ACS Macro Letters</i> , 2020 , 9, 1745-1752	6.6	10
105	Learning composition-transferable coarse-grained models: Designing external potential ensembles to maximize thermodynamic information. <i>Journal of Chemical Physics</i> , 2020 , 153, 154116	3.9	10
104	Mechanisms of Asymmetric Membrane Formation in Nonsolvent-Induced Phase Separation. <i>ACS Macro Letters</i> , 2020 , 9, 1617-1624	6.6	15

103	Theoretical prediction of an isotropic to nematic phase transition in bottlebrush homopolymer melts. <i>Journal of Chemical Physics</i> , 2019 , 151, 094901	3.9	8
102	Linear Scaling Self-Consistent Field Theory with Spectral Contour Accuracy. <i>ACS Macro Letters</i> , 2019 , 8, 1402-1406	6.6	6
101	Stability of the A15 phase in diblock copolymer melts. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 13194-13199	11.5	72
100	Optimized Phase Field Model for Diblock Copolymer Melts. <i>Macromolecules</i> , 2019 , 52, 2878-2888	5.5	7
99	Contrasting Dielectric Properties of Electrolyte Solutions with Polar and Polarizable Solvents. <i>Physical Review Letters</i> , 2019 , 122, 128007	7.4	11
98	Complete Phase Diagram for Liquid-Liquid Phase Separation of Intrinsically Disordered Proteins. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 1644-1652	6.4	128
97	Molecular design of self-coacervation phenomena in block polyampholytes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 8224-8232	11.5	66
96	Miktoarm Stars via Grafting-Through Copolymerization: Self-Assembly and the Star-to-Bottlebrush Transition. <i>Macromolecules</i> , 2019 , 52, 1794-1802	5.5	44
95	Field-Theoretic Study of Salt-Induced Order and Disorder in a Polarizable Diblock Copolymer. <i>ACS Macro Letters</i> , 2019 , 8, 962-967	6.6	18
94	Small ion effects on self-coacervation phenomena in block polyampholytes. <i>Journal of Chemical Physics</i> , 2019 , 151, 034904	3.9	33
93	Narrow equilibrium window for complex coacervation of tau and RNA under cellular conditions. <i>ELife</i> , 2019 , 8,	8.9	72
92	SCFT Study of Diblock Copolymer Melts in Electric Fields: Selective Stabilization of Orthorhombic Fddd Network Phase. <i>Macromolecules</i> , 2018 , 51, 3369-3378	5.5	9
91	Nucleation of the lamellar phase from the disordered phase of the renormalized Landau-Brazovskii model. <i>Journal of Chemical Physics</i> , 2018 , 148, 054903	3.9	4
90	Marangoni Flows during Nonsolvent Induced Phase Separation. <i>ACS Macro Letters</i> , 2018 , 7, 582-586	6.6	20
89	Field-theoretic simulations: An emerging tool for probing soft material assembly. <i>MRS Bulletin</i> , 2018 , 43, 371-378	3.2	10
88	Level-set strategy for inverse DSA-lithography. <i>Journal of Computational Physics</i> , 2018 , 375, 1159-1178	4.1	4
87	Coherent states field theory in supramolecular polymer physics. <i>Journal of Chemical Physics</i> , 2018 , 148, 204904	3.9	9
86	The effective χ parameter in polarizable polymeric systems: One-loop perturbation theory and field-theoretic simulations. <i>Journal of Chemical Physics</i> , 2018 , 148, 204903	3.9	17

85	QMCPACK: an open source ab initio quantum Monte Carlo package for the electronic structure of atoms, molecules and solids. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 195901	1.8	117
84	Theory of polyelectrolyte complexation-Complex coacervates are self-coacervates. <i>Journal of Chemical Physics</i> , 2017 , 146, 224902	3.9	99
83	Functional level-set derivative for a polymer self consistent field theory Hamiltonian. <i>Journal of Computational Physics</i> , 2017 , 345, 207-223	4.1	9
82	Effects of Tailored Dispersity on the Self-Assembly of Dimethylsiloxane-Methyl Methacrylate Block Co-Oligomers. <i>ACS Macro Letters</i> , 2017 , 6, 668-673	6.6	61
81	A multi-fluid model for microstructure formation in polymer membranes. <i>Soft Matter</i> , 2017 , 13, 3013-3030	3.6	34
80	A finite element approach to self-consistent field theory calculations of multiblock polymers. <i>Journal of Computational Physics</i> , 2017 , 331, 280-296	4.1	5
79	Orientalional Preference in Multilayer Block Copolymer Nanomeshes with Respect to Layer-to-Layer Commensurability. <i>Macromolecules</i> , 2017 , 50, 8258-8266	5.5	8
78	Inverse Design of Bulk Morphologies in Multiblock Polymers Using Particle Swarm Optimization. <i>Macromolecules</i> , 2017 , 50, 6702-6709	5.5	28
77	Optimized phase field models in confinement: fast and accurate simulations of directed self-assembly 2017 ,		3
76	Field-Theoretic Simulations of Fluctuation-Stabilized Aperiodic Bricks-and-Mortar Mesophase in Miktoarm Star Block Copolymer/Homopolymer Blends. <i>Macromolecules</i> , 2017 , 50, 6263-6272	5.5	11
75	Genetic Algorithm for Discovery of Globally Stable Phases in Block Copolymers. <i>Macromolecules</i> , 2016 , 49, 6558-6567	5.5	11
74	Recent Developments in Fully Fluctuating Field-Theoretic Simulations of Polymer Melts and Solutions. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 7615-34	3.4	71
73	Broadly Accessible Self-Consistent Field Theory for Block Polymer Materials Discovery. <i>Macromolecules</i> , 2016 , 49, 4675-4690	5.5	100
72	Fddd network phase in ABA triblock copolymer melts. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2016 , 54, 1112-1117	2.6	14
71	Cyclic Solvent Annealing Improves Feature Orientation in Block Copolymer Thin Films. <i>Macromolecules</i> , 2016 , 49, 1743-1751	5.5	20
70	Morphology re-entry in asymmetric PS-PI-PS' triblock copolymer and PS homopolymer blends. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2016 , 54, 169-179	2.6	6
69	Statistical field theory description of inhomogeneous polarizable soft matter. <i>Journal of Chemical Physics</i> , 2016 , 145, 154104	3.9	45
68	Cornucopia of Nanoscale Ordered Phases in Sphere-Forming Tetrablock Terpolymers. <i>ACS Nano</i> , 2016 , 10, 4961-72	16.7	79

67	Shape optimization for DSA 2016 ,		2
66	Phase field mapping for accurate, ultrafast simulations of directed self-assembly 2016 ,		3
65	Self-consistent field theory simulations of polymers on arbitrary domains. <i>Journal of Computational Physics</i> , 2016 , 327, 168-185	4.1	13
64	Swarm Intelligence Platform for Multiblock Polymer Inverse Formulation Design. <i>ACS Macro Letters</i> , 2016 , 5, 972-976	6.6	22
63	Aperiodic Bricks and Mortar Mesophase: a New Equilibrium State of Soft Matter and Application as a Stiff Thermoplastic Elastomer. <i>Macromolecules</i> , 2015 , 48, 5378-5384	5.5	27
62	Energy Transfer Directly to Bilayer Interfaces to Improve Exciton Collection in Organic Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 19011-19021	3.8	13
61	Creating Extremely Asymmetric Lamellar Structures via Fluctuation-Assisted Unbinding of Miktoarm Star Block Copolymer Alloys. <i>Journal of the American Chemical Society</i> , 2015 , 137, 6160-3	16.4	33
60	Effects of thermal fluctuations on directed self-assembly in cylindrical confinement. <i>Journal of Micro/ Nanolithography, MEMS, and MOEMS</i> , 2015 , 14, 013505	0.7	3
59	Computational study of directed self-assembly for contact-hole shrink and multiplication. <i>Journal of Micro/ Nanolithography, MEMS, and MOEMS</i> , 2015 , 14, 013501	0.7	3
58	First-principles calculations of indirect Auger recombination in nitride semiconductors. <i>Physical Review B</i> , 2015 , 92,	3.3	57
57	Field-theoretic Simulations of Directed Self-assembly for Contact Multiplication. <i>Journal of Photopolymer Science and Technology = [Fotopolyma Konwakai Shi]</i> , 2015 , 28, 689-693	0.7	5
56	Truncation-based energy weighting string method for efficiently resolving small energy barriers. <i>Journal of Chemical Physics</i> , 2015 , 143, 054105	3.9	14
55	Advantages and limitations of density functional theory in block copolymer directed self-assembly 2015 ,		1
54	Directed self-assembly of linear arrays of block copolymer cylinders. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2015 , 53, 317-326	2.6	9
53	Self-consistent field theory investigation of directed self-assembly in cylindrical confinement. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2015 , 53, 142-153	2.6	26
52	Computational Study of Directed Self-Assembly in Neutral Prepatterns for a Graphoepitaxial Pitch-Multiplication Application. <i>Macromolecules</i> , 2015 , 48, 1256-1261	5.5	8
51	Landau theory of topological defects in multiferroic hexagonal manganites. <i>Nature Materials</i> , 2014 , 13, 42-9	27	128
50	Block Copolymer Self Assembly during Rapid Solvent Evaporation: Insights into Cylinder Growth and Stability. <i>ACS Macro Letters</i> , 2014 , 3, 16-20	6.6	76

49	Improving brush polymer infrared one-dimensional photonic crystals via linear polymer additives. <i>Journal of the American Chemical Society</i> , 2014 , 136, 17374-7	16.4	103
48	Phase Coexistence Calculations of Reversibly Bonded Block Copolymers: A Unit Cell Gibbs Ensemble Approach. <i>Macromolecules</i> , 2014 , 47, 1865-1874	5.5	10
47	Improving Energy Relay Dyes for Dye Sensitized Solar Cells by Increasing Donor Homotransfer. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 14098-14106	3.8	9
46	Field-Theoretic Simulations of Multi-Cylinder Configurations in VIA Lithography. <i>Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi]</i> , 2014 , 27, 21-24	0.7	7
45	The Hole Shrink Problem: Self-Consistent Field Theory for Directed Self-Assembly of Miktoarm Copolymers. <i>Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi]</i> , 2014 , 27, 37-39	0.7	7
44	Field-theoretic simulations of directed self-assembly in cylindrical confinement: placement and rectification aspects 2014 ,		6
43	Directed self-assembly of diblock copolymers in laterally confining channels: line-edge-roughness and defectivity 2014 ,		3
42	Computational studies of shape rectification in directed self-assembly 2014 ,		1
41	Self-consistent field theory of directed self-assembly on chemically prepatterned surfaces 2014 ,		4
40	A multi-species exchange model for fully fluctuating polymer field theory simulations. <i>Journal of Chemical Physics</i> , 2014 , 141, 174103	3.9	39
39	Thermodynamic and kinetic aspects of defectivity in directed self-assembly of cylinder-forming diblock copolymers in laterally confining thin channels. <i>Journal of Applied Polymer Science</i> , 2014 , 131, n/a-n/a	2.9	26
38	Coherent states formulation of polymer field theory. <i>Journal of Chemical Physics</i> , 2014 , 140, 024905	3.9	13
37	Comparison of Pseudospectral Algorithms for Field-Theoretic Simulations of Polymers. <i>Macromolecules</i> , 2013 , 46, 8383-8391	5.5	24
36	Quantification of octahedral rotations in strained LaAlO ₃ films via synchrotron x-ray diffraction. <i>Physical Review B</i> , 2013 , 88,	3.3	35
35	Polymer field-theory simulations on graphics processing units. <i>Computer Physics Communications</i> , 2013 , 184, 2102-2110	4.2	37
34	Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially strained orthorhombic LaMnO ₃ . <i>Physical Review B</i> , 2013 , 88,	3.3	67
33	Striped, ellipsoidal particles by controlled assembly of diblock copolymers. <i>Journal of the American Chemical Society</i> , 2013 , 135, 6649-57	16.4	180
32	The hole shrink problem: Theoretical studies of directed self-assembly in cylindrical confinement 2013 ,		12

31	Structural and optoelectronic characterization of RF sputtered ZnSnN(2). <i>Advanced Materials</i> , 2013 , 25, 2562-6	24	129
30	Poster: Spin-Related Phenomena 2013 , 589-632		
29	The Hole Shrink Problem: Directed Self-Assembly Using Self-Consistent Field Theory. <i>Journal of Photopolymer Science and Technology = [Fotoporima Konwakai Shi]</i> , 2013 , 26, 15-20	0.7	16
28	Defectivity in Laterally Confined Lamella-Forming Diblock Copolymers: Thermodynamic and Kinetic Aspects. <i>Macromolecules</i> , 2012 , 45, 6253-6265	5.5	122
27	Reactivity ratios, and mechanistic insight for anionic ring-opening copolymerization of epoxides. <i>Macromolecules</i> , 2012 , 45, 3722-3731	5.5	43
26	Multiblock polymers: panacea or Pandora's box?. <i>Science</i> , 2012 , 336, 434-40	33.3	77 ⁸
25	Scaling Behavior and Beyond Equilibrium in the Hexagonal Manganites. <i>Physical Review X</i> , 2012 , 2,	9.1	88
24	Anisotropic conductance at improper ferroelectric domain walls. <i>Nature Materials</i> , 2012 , 11, 284-8	27	347
23	Low-temperature ketene formation in materials chemistry through molecular engineering. <i>Chemical Science</i> , 2012 , 3, 766-771	9.4	27
22	Earth-abundant ZnSn _x Ge _{1-x} N ₂ alloys as potential photovoltaic absorber materials 2012 ,		4
21	Self-consistent field theory of directed self-assembly in laterally confined lamellae-forming diblock copolymers 2012 ,		7
20	Indirect Auger recombination as a cause of efficiency droop in nitride light-emitting diodes. <i>Applied Physics Letters</i> , 2011 , 98, 161107	3.4	388
19	Local density of states and interface effects in semimetallic ErAs nanoparticles embedded in GaAs. <i>Physical Review Letters</i> , 2011 , 107, 036806	7.4	24
18	Unexpectedly large electronic contribution to linear magnetoelectricity. <i>Physical Review Letters</i> , 2011 , 106, 107202	7.4	46
17	Unusual dielectric response in B-site size-disordered hexagonal transition metal oxides. <i>Applied Physics Letters</i> , 2010 , 96, 162903	3.4	12
16	Theoretical study of Schottky-barrier formation at epitaxial rare-earth-metal/semiconductor interfaces. <i>Physical Review B</i> , 2010 , 81,	3.3	30
15	Temperature-dependent magnetoelectric effect from first principles. <i>Physical Review Letters</i> , 2010 , 105, 087202	7.4	69
14	Electric and magnetic polarizabilities of hexagonal Ln ₂ CuTiO ₆ (Ln=Y, Dy, Ho, Er, and Yb). <i>Physical Review B</i> , 2010 , 82,	3.3	16

13	Electrical conductivity of high-pressure liquid hydrogen by quantum Monte Carlo methods. <i>Physical Review Letters</i> , 2009 , 103, 256401	7.4	26
12	Role of atomic multiplets in the electronic structure of rare-earth semiconductors and semimetals. <i>Physical Review Letters</i> , 2009 , 102, 096401	7.4	23
11	Superexchange-driven magnetoelectricity in magnetic vortices. <i>Physical Review Letters</i> , 2009 , 102, 157203	7.4	46
10	Mn ³⁺ in trigonal bipyramidal coordination: a new blue chromophore. <i>Journal of the American Chemical Society</i> , 2009 , 131, 17084-6	16.4	117
9	Auger recombination rates in nitrides from first principles. <i>Applied Physics Letters</i> , 2009 , 94, 191109	3.4	297
8	Near-infrared absorption and semimetal-semiconductor transition in 2nm ErAs nanoparticles embedded in GaAs and AlAs. <i>Applied Physics Letters</i> , 2008 , 92, 173116	3.4	22
7	Theoretical study of the structural and electronic properties of strained ErAs. <i>Physical Review B</i> , 2008 , 77,	3.3	11
6	Trial wave functions for high-pressure metallic hydrogen. <i>Computer Physics Communications</i> , 2008 , 179, 89-97	4.2	19
5	Vertex corrections in localized and extended systems. <i>Physical Review B</i> , 2007 , 76,	3.3	40
4	Quantum Monte Carlo simulation of the high-pressure molecular-atomic crossover in fluid hydrogen. <i>Physical Review Letters</i> , 2006 , 97, 235702	7.4	57
3	Image states in metal clusters. <i>Physical Review A</i> , 2004 , 70,	2.6	32
2	Comment on "band-gap problem in semiconductors revisited: effects of core States and many-body self-consistency". <i>Physical Review Letters</i> , 2004 , 93, 249701; author reply 249702	7.4	59
1	Narrow equilibrium window for complex coacervation of tau and RNA under cellular conditions		4