Fernando A Escobedo

List of Publications by Year
in descending order

164 papers	5,580 citations	61984 43 h-index	102487 66 g-index
164 all docs	164 docs citations	164 times ranked	4265 citing authors

#	Article	IF	Citations
1	On the simulation of vaporâ€"liquid equilibria for alkanes. Journal of Chemical Physics, 1998, 108, 9905-9911.	3.0	418
2	Mesophase behaviour of polyhedral particles. Nature Materials, 2011, 10, 230-235.	27.5	278
3	Expanded grand canonical and Gibbs ensemble Monte Carlo simulation of polymers. Journal of Chemical Physics, 1996, 105, 4391-4394.	3.0	194
4	Extended continuum configurational bias Monte Carlo methods for simulation of flexible molecules. Journal of Chemical Physics, 1995, 102, 2636-2652.	3.0	123
5	Monte Carlo simulation of the chemical potential of polymers in an expanded ensemble. Journal of Chemical Physics, 1995, 103, 2703-2710.	3.0	110
6	Phase behavior of rounded hard-squares. Soft Matter, 2012, 8, 4675.	2.7	104
7	Revealing the atomic ordering of binary intermetallics using in situ heating techniques at multilength scales. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1974-1983.	7.1	98
8	SIMULATION OFPHASETRANSITIONS INFLUIDS. Annual Review of Physical Chemistry, 1999, 50, 377-411.	10.8	94
9	Simulation and prediction of vapour-liquid equilibria for chain molecules. Molecular Physics, 1996, 87, 347-366.	1.7	90
10	Phase behavior of colloidal hard perfect tetragonal parallelepipeds. Journal of Chemical Physics, 2008, 128, 044909.	3.0	90
11	Influence of Side-Chain Chemistry on Structure and Ionic Conduction Characteristics of Polythiophene Derivatives: A Computational and Experimental Study. Chemistry of Materials, 2019, 31, 1418-1429.	6.7	84
12	Simulation of the gyroid phase in off-lattice models of pure diblock copolymer melts. Journal of Chemical Physics, 2006, 125, 104907.	3.0	82
13	Reaction coordinates and transition pathways of rare events via forward flux sampling. Journal of Chemical Physics, 2007, 127, 164101.	3.0	81
14	Molecular Simulations of Wetting of a Rough Surface by an Oily Fluid: Effect of Topology, Chemistry, and Droplet Size on Wetting Transition Rates. Langmuir, 2012, 28, 3412-3419.	3.5	72
15	Cubatic liquid-crystalline behavior in a system of hard cuboids. Journal of Chemical Physics, 2004, 120, 9383-9389.	3.0	71
16	Phase Behavior of Colloidal Hard Tetragonal Parallelepipeds (Cuboids):Â A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2005, 109, 23008-23015.	2.6	70
17	Monte Carlo simulation of branched and crosslinked polymers. Journal of Chemical Physics, 1996, 104, 4788-4801.	3.0	69
18	Novel pseudoensembles for simulation of multicomponent phase equilibria. Journal of Chemical Physics, 1998, 108, 8761-8772.	3.0	69

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19	Molecular simulation of polymeric networks and gels: phase behavior and swelling. Physics Reports, 1999, 318, 85-112.	25.6	69
20	Monte Carlo simulation of athermal mesogenic chains: Pure systems, mixtures, and constrained environments. Journal of Chemical Physics, 1997, 106, 9858-9868.	3.0	68
21	Transition path sampling and forward flux sampling. Applications to biological systems. Journal of Physics Condensed Matter, 2009, 21, 333101.	1.8	67
22	Molecular dynamics simulation of the mesophase behaviour of a model bolaamphiphilic liquid crystal with a lateral flexible chain. Soft Matter, 2008, 4, 1820.	2.7	65
23	Thermodynamics and kinetics of bubble nucleation: Simulation methodology. Journal of Chemical Physics, 2012, 137, 074109.	3.0	65
24	Single polymer growth dynamics. Science, 2017, 358, 352-355.	12.6	65
25	Simulation Study of Free-Energy Barriers in the Wetting Transition of an Oily Fluid on a Rough Surface with Reentrant Geometry. Langmuir, 2012, 28, 16080-16090.	3.5	63
26	Molecular Dynamics of Equilibrium and Pressure-Driven Transport Properties of Water through LTA-Type Zeolites. Langmuir, 2013, 29, 12389-12399.	3.5	62
27	Lattice Monte Carlo Simulations of the Gyroid Phase in Monodisperse and Bidisperse Block Copolymer Systems. Macromolecules, 2005, 38, 8522-8531.	4.8	59
28	Structure and transport properties of polymer grafted nanoparticles. Journal of Chemical Physics, 2011, 135, 184902.	3.0	59
29	A configurational-bias approach for the simulation of inner sections of linear and cyclic molecules. Journal of Chemical Physics, 2000, 113, 11382-11392.	3.0	58
30	Simulation and theory of the swelling of athermal gels. Journal of Chemical Physics, 1997, 106, 793-810.	3.0	57
31	Optimizing the sampling and staging for simulations of rare events via forward flux sampling schemes. Journal of Chemical Physics, 2008, 129, 024115.	3.0	55
32	Synthesis and assembly of nonspherical hollow silica colloids under confinement. Journal of Materials Chemistry, 2008, 18, 4912.	6.7	52
33	Optimization of expanded ensemble methods. Journal of Chemical Physics, 2008, 129, 154107.	3.0	51
34	Bicontinuous Phases in Diblock Copolymer/Homopolymer Blends: Simulation and Self-Consistent Field Theory. Macromolecules, 2009, 42, 1775-1784.	4.8	51
35	On the use of Bennettâ€™s acceptance ratio method in multi-canonical-type simulations. Journal of Chemical Physics, 2004, 120, 3066-3074.	3.0	49
36	Chemical potential and equations of state of hard core chain molecules. Journal of Chemical Physics, 1995, 103, 1946-1956.	3.0	48

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37	Simulation of Vaporâ"Liquid Equilibria for Alkane Mixtures. Industrial & Engineering Chemistry Research, 1998, 37, 3195-3202.	3.7	47
38	Molecular simulations in chemical engineering: Present and future. AICHE Journal, 2002, 48, 2716-2721.	3.6	46
39	Expanded ensemble and replica exchange methods for simulation of protein-like systems. Journal of Chemical Physics, 2003, 119, 11998-12010.	3.0	46
40	Effect of shear on nanoparticle dispersion in polymer melts: A coarse-grained molecular dynamics study. Journal of Chemical Physics, 2010, 132, 024901.	3.0	46
41	Characterizing the Structural Behavior of Selected AÎ²-42 Monomers with Different Solubilities. Journal of Physical Chemistry B, 2011, 115, 4900-4910.	2.6	45
42	Engineering entropy in soft matter: the bad, the ugly and the good. Soft Matter, 2014, 10, 8388-8400.	2.7	45
43	Monte Carlo Simulation of the Effect of Entanglements on the Swelling and Deformation Behavior of End-Linked Polymeric Networks. Macromolecules, 2002, 35, 3296-3305.	4.8	44
44	Optimized expanded ensembles for simulations involving molecular insertions and deletions. I. Closed systems. Journal of Chemical Physics, 2007, 127, 174103.	3.0	44
45	Simulation of Isoenthalps and Joule-Thomson Inversion Curves of Pure Fluids and Mixtures. Molecular Simulation, 2001, 26, 395-416.	2.0	41
46	Monte Carlo Study of the Stabilization of Complex Bicontinuous Phases in Diblock Copolymer Systems. Macromolecules, 2007, 40, 7354-7365.	4.8	39
47	Experiments and Simulations: Enhanced Mechanical Properties of End-Linked Bimodal Elastomers. Macromolecules, 2008, 41, 8231-8241.	4.8	39
48	Assembly of porous smectic structures formed from interlocking high-symmetry planar nanorings. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9699-9703.	7.1	39
49	Coarse-grained molecular dynamics simulation on the placement of nanoparticles within symmetric diblock copolymers under shear flow. Journal of Chemical Physics, 2008, 128, 164909.	3.0	38
50	The Plumberâ€™s Nightmare Phase in Diblock Copolymer/Homopolymer Blends. A Self-Consistent Field Theory Study.. Macromolecules, 2009, 42, 9058-9062.	4.8	38
51	Pseudo-ensemble simulations and Gibbsâ€"Duhem integrations for polymers. Journal of Chemical Physics, 1997, 106, 2911-2923.	3.0	37
52	Rotator and crystalline films viaself-assembly of short-bond-length colloidal dimers. Journal of Materials Chemistry, 2009, 19, 344-349.	6.7	37
53	Tracing coexistence lines in multicomponent fluid mixtures by molecular simulation. Journal of Chemical Physics, 1999, 110, 11999-12010.	3.0	36
54	Packing, entropic patchiness, and self-assembly of non-convex colloidal particles: A simulation perspective. Current Opinion in Colloid and Interface Science, 2017, 30, 62-69.	7.4	36

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55	Complex Relationship between Side-Chain Polarity, Conductivity, and Thermal Stability in Molecularly Doped Conjugated Polymers. Chemistry of Materials, 2021, 33, 741-753.	6.7	36
56	Glassy Dislocation Dynamics in 2D Colloidal Dimer Crystals. Physical Review Letters, 2010, 105, 078301.	7.8	35
57	Computational affinity maturation of camelid single-domain intrabodies against the nonamyloid component of alpha-synuclein. Scientific Reports, 2018, 8, 17611.	3.3	35
58	A general framework for non-Boltzmann Monte Carlo sampling. Journal of Chemical Physics, 2006, 124, 054116.	3.0	33
59	Kinetics and mechanism of the unfolding native-to-loop transition of Trp-cage in explicit solvent via optimized forward flux sampling simulations. Journal of Chemical Physics, 2010, 133, 105103.	3.0	32
60	Monte Carlo simulation of polymer chain collapse in an athermal solvent. Journal of Chemical Physics, 1997, 106, 1288-1290.	3.0	31
61	Computation of Free Energies of Cubic Bicontinuous Phases for Blends of Diblock Copolymer and Selective Homopolymer. Macromolecules, 2016, 49, 5232-5243.	4.8	30
62	Localized Orientational Order Chaperones the Nucleation of Rotator Phases in Hard Polyhedral Particles. Physical Review Letters, 2014, 112, 048301.	7.8	29
63	Structure Control of a Ï€-Conjugated Oligothiophene-Based Liquid Crystal for Enhanced Mixed Ion/Electron Transport Characteristics. ACS Nano, 2019, 13, 7665-7675.	14.6	29
64	On the use of transition matrix methods with extended ensembles. Journal of Chemical Physics, 2006, 124, 104110.	3.0	28
65	Effect of quenched size polydispersity on the ordering transitions of hard polyhedral particles. Journal of Chemical Physics, 2012, 137, 024905.	3.0	28
66	Chemical potential and dimensions of chain molecules in athermal environments. Molecular Physics, 1996, 89, 1733-1754.	1.7	28
67	Simulation of bulk, confined, and polydisperse systems. I. A unified methodological framework. Journal of Chemical Physics, 2001, 115, 5642-5652.	3.0	27
68	Optimized expanded ensembles for simulations involving molecular insertions and deletions. II. Open systems. Journal of Chemical Physics, 2007, 127, 174104.	3.0	27
69	Mesoscopic structure prediction of nanoparticle assembly and coassembly: Theoretical foundation. Journal of Chemical Physics, 2010, 133, 194108.	3.0	26
70	Folding kinetics of a lattice protein via a forward flux sampling approach. Journal of Chemical Physics, 2006, 125, 164904.	3.0	25
71	Side chain engineering control of mixed conduction in oligoethylene glycol-substituted polythiophenes. Journal of Materials Chemistry A, 2021, 9, 21410-21423.	10.3	25
72	Self-assembly of binary space-tessellating compounds. Journal of Chemical Physics, 2012, 137, 194907.	3.0	24

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73	Predicting Chiral Nanostructures, Lattices and Superlattices in Complex Multicomponent Nanoparticle Self-Assembly. Nano Letters, 2012, 12, 3218-3223.	9.1	24
74	Phase behavior of binary mixtures of hard convex polyhedra. Soft Matter, 2013, 9, 11557.	2.7	24
75	Phase behavior of polyhedral nanoparticles in parallel plate confinement. Soft Matter, 2016, 12, 1506-1516.	2.7	24
76	Correlation between Ionic Mobility and Microstructure in Block Copolymers. A Coarse-Grained Modeling Study. Macromolecules, 2018, 51, 9213-9221.	4.8	23
77	Simulation and extrapolation of coexistence properties with single-phase and two-phase ensembles. Journal of Chemical Physics, 2000, 113, 8444-8456.	3.0	22
78	Hybrid Monte Carlo with multidimensional replica exchanges: Conformational equilibria of the hypervariable regions of a llama VHH antibody domain. Biopolymers, 2003, 68, 160-177.	2.4	22
79	Liquid crystalline behavior of a semifluorinated oligomer. Journal of Chemical Physics, 2004, 121, 11463.	3.0	22
80	Directed self-assembly of spherical caps via confinement. Soft Matter, 2013, 9, 9153.	2.7	22
81	Multicanonical schemes for mapping out free-energy landscapes of single-component and multicomponent systems. Journal of Chemical Physics, 2005, 122, 164103.	3.0	21
82	Protein translocation through a tunnel induces changes in folding kinetics: A lattice model study. Biotechnology and Bioengineering, 2006, 94, 105-117.	3.3	21
83	Variance Minimization of Free Energy Estimates from Optimized Expanded Ensembles. Journal of Physical Chemistry B, 2008, 112, 8120-8128.	2.6	21
84	Simulation of Chain-length Partitioning in a Microfabricated Channel via Entropic Trapping. Molecular Simulation, 2003, 29, 417-425.	2.0	20
85	Simulating the Kinetics and Thermodynamics of Transitions via Forward Flux/Umbrella Sampling. Journal of Physical Chemistry B, 2009, 113, 6434-6445.	2.6	20
86	Simultaneous estimation of free energies and rates using forward flux sampling and mean first passage times. Journal of Chemical Physics, 2015, 143, 244113.	3.0	20
87	Entropic self-assembly of freely rotating polyhedral particles confined to a flat interface. Soft Matter, 2015, 11, 1481-1491.	2.7	20
88	Selfâ€Assembly Behavior of an Oligothiopheneâ€Based Conjugated Liquid Crystal and Its Implication for Ionic Conductivity Characteristics. Advanced Functional Materials, 2019, 29, 1805220.	14.9	20
89	A new method for generating volume changes in isobaric-isothermal Monte Carlo simulations of flexible molecules. Macromolecular Theory and Simulations, 1995, 4, 691-707.	1.4	19
90	Simulation of swelling of model polymeric gels by subcritical and supercritical solvents. Journal of Chemical Physics, 1999, 110, 1290-1298.	3.0	19

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91	Conformational Properties and Entropic Partitioning of Topologically Complex Polymers under Confinement. Macromolecules, 2001, 34, 8802-8810.	4.8	19
92	Influence of polymer architecture and polymer-wall interaction on the adsorption of polymers into a slit-pore. Physical Review E, 2004, 69, 021802.	2.1	19
93	Sawtooth Tensile Response of Model Semiflexible and Block Copolymer Elastomers. Macromolecules, 2014, 47, 840-850.	4.8	19
94	A novel algorithm for characterization of order in materials. Journal of Chemical Physics, 2002, 117, 4000-4009.	3.0	18
95	A Novel Configurational-Bias Monte Carlo Method for Lattice Polymers:Â Application to Molecules with Multicyclic Architectures. Macromolecules, 2005, 38, 8532-8545.	4.8	18
96	A theoretical and simulation study of the self-assembly of a binary blend of diblock copolymers. Journal of Chemical Physics, 2012, 136, 234905.	3.0	18
97	Mechanical Properties of Tetrapolyethylene and Tetrapoly(ethylene oxide) Diamond Networks via Molecular Dynamics Simulations. Macromolecules, 2016, 49, 2375-2386.	4.8	18
98	Molecular dynamics simulation of thermotropic bolaamphiphiles with a swallow-tail lateral chain: formation of cubic network phases. Soft Matter, 2017, 13, 8542-8555.	2.7	18
99	Far-from-equilibrium sheared colloidal liquids: Disentangling relaxation, advection, and shear-induced diffusion. Physical Review E, 2013, 88, 062309.	2.1	17
100	Mapping coexistence lines via free-energy extrapolation: Application to order-disorder phase transitions of hard-core mixtures. Journal of Chemical Physics, 2014, 140, 094102.	3.0	17
101	A unified methodological framework for the simulation of nonisothermal ensembles. Journal of Chemical Physics, 2005, 123, 044110.	3.0	16
102	STUDY OF SOLID-LIQUID EXTRACTIONS IN A BATCH EQUIPMENT. Chemical Engineering Communications, 1998, 167, 73-86.	2.6	15
103	Formation and Characterization of Semiflexible Polymer Networks via Monte Carlo Simulations. Macromolecules, 2004, 37, 3924-3933.	4.8	15
104	Diffusivities and Viscosities of Poly(ethylene oxide) Oligomers. Journal of Chemical & Engineering Data, 2010, 55, 4273-4280.	1.9	15
105	Nucleus-size pinning for determination of nucleation free-energy barriers and nucleus geometry. Journal of Chemical Physics, 2018, 148, 184104.	3.0	15
106	On the Scaling of the Critical Solution Temperature of Binary Polymer Blends with Chain Length. Macromolecules, 1999, 32, 900-910.	4.8	14
107	A simulation study of lyotropic isotropicâ€"nematic phase transitions in polydisperse chain systems. Journal of Chemical Physics, 2003, 118, 10262-10275.	3.0	14
108	Heuristic Rule for Binary Superlattice Coassembly: Mixed Plastic Mesophases of Hard Polyhedral Nanoparticles. Physical Review Letters, 2014, 113, 165504.	7.8	14

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109	Molecular and macroscopic modeling of phase separation. AICHE Journal, 2000, 46, 2086-2096.	3.6	13
110	Simulation of bulk, confined, and polydisperse systems. II. Application to chain systems. Journal of Chemical Physics, 2001, 115, 5653-5661.	3.0	13
111	Developing Local Order Parameters for Orderâ€"Disorder Transitions From Particles to Block Copolymers: Application to Macromolecular Systems. Macromolecules, 2018, 51, 9781-9788.	4.8	13
112	²H NMR and Simulation Studies of Chain Segment Orientation in PDMS Bimodal Networks. Macromolecules, 2010, 43, 7173-7184.	4.8	12
113	Degenerate crystals from colloidal dimers under confinement. Soft Matter, 2014, 10, 9729-9738.	2.7	12
114	Extensions of the interfacial pinning method and application to hard core systems. Journal of Chemical Physics, 2014, 141, 124117.	3.0	12
115	Optimizing the formation of colloidal compounds with components of different shapes. Journal of Chemical Physics, 2017, 147, 214501.	3.0	12
116	Developing Local Order Parameters for Orderâ€"Disorder Transitions From Particles to Block Copolymers: Methodological Framework. Macromolecules, 2018, 51, 9769-9780.	4.8	12
117	Phase behaviour of model polymeric networks and gels. Molecular Physics, 1997, 90, 437-443.	1.7	12
118	Simulation and prediction of vapour-liquid equilibria for chain molecules. Molecular Physics, 1996, 87, 347-366.	1.7	11
119	Simulation of the density of states in isothermal and adiabatic ensembles. Physical Review E, 2006, 73, 056701.	2.1	10
120	Tuning the Sawtooth Tensile Response and Toughness of Multiblock Copolymer Diamond Networks. Macromolecules, 2016, 49, 6711-6721.	4.8	10
121	Solid-phase nucleation free-energy barriers in truncated cubes: interplay of localized orientational order and facet alignment. Soft Matter, 2018, 14, 1996-2005.	2.7	10
122	On the application of virtual Gibbs ensembles to the direct simulation of fluidâ€"fluid and solidâ€"fluid phase coexistence. Journal of Chemical Physics, 2002, 116, 7957-7966.	3.0	9
123	Stepwise Elastic Behavior in a Model Elastomer. Physical Review Letters, 2004, 93, 257804.	7.8	9
124	Monte Carlo Simulation of the Topology and Conformational Behavior of Hyperbranched Molecules: Pd-Diimine-Catalyzed Polyethylene. Macromolecular Theory and Simulations, 2002, 11, 136-146.	1.4	8
125	Tilting the Balance between Canonical and Noncanonical Conformations for the H1 Hypervariable Loop of a Llama VHH through Point Mutations. Journal of Physical Chemistry B, 2013, 117, 13-24.	2.6	8
126	Effect of inter-species selective interactions on the thermodynamics and nucleation free-energy barriers of a tessellating polyhedral compound. Journal of Chemical Physics, 2016, 145, 211903.	3.0	8

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127	Optimizing the network topology of block copolymer liquid crystal elastomers for enhanced extensibility and toughness. Physical Review Materials, 2017, 1, .	2.4	8
128	Gibbs-Duhem integration in lattice systems. Europhysics Letters, 1997, 40, 111-116.	2.0	7
129	Bridging continuum and statistical thermodynamics via equations of state and the density of states. Journal of Chemical Physics, 2004, 120, 10699-10710.	3.0	7
130	In Silico Protein Fragmentation Reveals the Importance of Critical Nuclei on Domain Reassembly. Biophysical Journal, 2008, 94, 1575-1588.	0.5	7
131	Exploration of Factors Affecting the Onset and Maturation Course of Follicular Lymphoma through Simulations ofÂtheÂGerminal Center. Bulletin of Mathematical Biology, 2009, 71, 1432-1462.	1.9	7
132	Kinetics and Reaction Coordinates of the Reassembly of Protein Fragments Via Forward Flux Sampling. Biophysical Journal, 2010, 98, 1911-1920.	0.5	7
133	Transport Properties of Amine/Carbon Dioxide Reactive Mixtures and Implications to Carbon Capture Technologies. ACS Applied Materials & Interfaces, 2015, 7, 17603-17613.	8.0	7
134	Heat capacities of supercritical fluid mixtures: Comparing experimental measurements with Monte Carlo molecular simulations for carbon dioxide-methanol mixtures. Journal of Supercritical Fluids, 2017, 123, 40-49.	3.2	7
135	Creating microenvironments using encapsulated polymers. Journal of Polymer Science Part A, 2008, 46, 2309-2315.	2.3	6
136	Extraction of Segment Orientation Distributions in Polymer Networks by Inversion of²H NMR Spectra through the Maximum-Entropy Method. Macromolecules, 2009, 42, 8889-8898.	4.8	6
137	Phase behaviour of PMMA-b-PHEMA with solvents methanol and THF: modelling and comparison to the experiment. Soft Matter, 2014, 10, 6172-6181.	2.7	6
138	Optimizing the formation of solid solutions with components of different shapes. Journal of Chemical Physics, 2017, 146, 134508.	3.0	6
139	Disorder Foreshadows Order in Colloidal Cubes. Journal of Physical Chemistry B, 2018, 122, 9264-9273.	2.6	6
140	Correlation between morphology and anisotropic transport properties of diblock copolymers melts. Soft Matter, 2019, 15, 851-859.	2.7	6
141	Bridging hexatic and tetratic phases in binary mixtures through near critical point fluctuations. Physical Review Materials, 2021, 5, .	2.4	6
142	Modeling the orientational and positional behavior of polyhedral nanoparticles at fluid-fluid interfaces. Physical Review Materials, 2017, 1, .	2.4	6
143	Simulated Mutagenesis of the Hypervariable Loops of a Llama VHH Domain for the Recovery of Canonical Conformations. Journal of Physical Chemistry B, 2009, 113, 1785-1795.	2.6	5
144	Swelling and Tensile Properties of Tetraâ€Polyethylene glycol via Coarseâ€Grained Molecular Models. Macromolecular Theory and Simulations, 2017, 26, 1600098.	1.4	5

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145	An Implicit-Solvent Model for the Interfacial Configuration of Colloidal Nanoparticles and Application to the Self-Assembly of Truncated Cubes. Journal of Chemical Theory and Computation, 2020, 16, 5866-5875.	5.3	5
146	Monte Carlo Methods for Polymeric Systems. Advances in Chemical Physics, 0, , 337-367.	0.3	5
147	Ligand Interactions and Nanoparticle Shapes Guide the Pathways toward Interfacial Self-Assembly. Langmuir, 2022, 38, 1738-1747.	3.5	5
148	Reaction Fronts in a Porous Medium. Approximation Techniques versus Numerical Solution. Industrial & Engineering Chemistry Research, 1995, 34, 794-805.	3.7	4
149	Yielding and shear induced melting of 2D mixed crystals of spheres and dimers. Soft Matter, 2012, 8, 5916.	2.7	4
150	Framework for Inverse Mapping Chemistry-Agnostic Coarse-Grained Simulation Models into Chemistry-Specific Models. Journal of Chemical Information and Modeling, 2019, 59, 5045-5056.	5.4	4
151	Molecular simulation of the effects of humidity and of interfacial Si- and B-hydroxyls on the adhesion energy between glass plates. Journal of Colloid and Interface Science, 2016, 465, 233-241.	9.4	3
152	Heat capacities of supercritical fluids via Grand Canonical ensemble simulations. Molecular Simulation, 2018, 44, 147-155.	2.0	3
153	Stability of the Gyroid Phase in Rodâ€"Coil Systems via Thermodynamic Integration with Molecular Dynamics. Journal of Chemical Theory and Computation, 2018, 14, 5984-5991.	5.3	3
154	Molecular Simulations of Laser Spike Annealing of Block Copolymer Lamellar Thin-Films. Langmuir, 2020, 36, 5754-5764.	3.5	3
155	Simulation of chain molecules for prediction of thermodynamic properties. Fluid Phase Equilibria, 1996, 116, 312-319.	2.5	2
156	Probability density of macrostates and density of states for multi-component mixtures from semi-empirical equations of state. Molecular Physics, 2005, 103, 3115-3124.	1.7	2
157	Effect of Block Immiscibility on Strain-Induced Microphase Segregation and Crystallization of Model Block Copolymer Elastomers. Macromolecules, 2018, 51, 5685-5693.	4.8	2
158	Thermal Stability of Ï€-Conjugated n-Ethylene-Glycol-Terminated Quaterthiophene Oligomers: A Computational and Experimental Study. ACS Macro Letters, 2020, 9, 295-300.	4.8	2
159	Topological Frustration as a New Parameter to Tune Morphology Revealed through Exploring the Continuum between A-B-C 3-Arm Star and Linear Triblock Polymers. Macromolecules, 2021, 54, 4401-4411.	4.8	2
160	Low Interfacial Free Energy Describes the Bulk Ordering Transition in Colloidal Cubes. Journal of Physical Chemistry B, 2021, 125, 5160-5170.	2.6	2
161	Congruent phase behavior of a binary compound crystal of colloidal spheres and dimpled cubes. Journal of Chemical Physics, 2020, 153, 214503.	3.0	2
162	Computing free energy barriers for the nucleation of complex network mesophases. Journal of Chemical Physics, 2022, 156, 034502.	3.0	2

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163	On the calculation of free energies over Hamiltonian and order parameters via perturbation and thermodynamic integration. Journal of Chemical Physics, 2021, 155, 114112.	3.0	1
164	Re-entrant transition as a bridge of broken ergodicity in confined monolayers of hexagonal prisms and cylinders. Journal of Colloid and Interface Science, 2022, 607, 1478-1490.	9.4	1