Fernando A Escobedo

List of Publications by Citations

163 papers	4,868 citations	41 h-index	61 g-index
164 ext. papers	5,216 ext. citations	4.9 avg, IF	6.08 L-index

#	Paper	IF	Citations
163	On the simulation of vapor□liquid equilibria for alkanes. *Journal of Chemical Physics*, **1998**, 108, 9905-9911	3.9	378
162	Mesophase behaviour of polyhedral particles. *Nature Materials*, **2011**, 10, 230-5	27	242
161	Expanded grand canonical and Gibbs ensemble Monte Carlo simulation of polymers. *Journal of Chemical Physics*, **1996**, 105, 4391-4394	3.9	181
160	Extended continuum configurational bias Monte Carlo methods for simulation of flexible molecules. *Journal of Chemical Physics*, **1995**, 102, 2636-2652	3.9	115
159	Monte Carlo simulation of the chemical potential of polymers in an expanded ensemble. *Journal of Chemical Physics*, **1995**, 103, 2703-2710	3.9	100
158	Simulation of phase transitions in fluids. *Annual Review of Physical Chemistry*, **1999**, 50, 377-411	15.7	87
157	Phase behavior of rounded hard-squares. *Soft Matter*, **2012**, 8, 4675	3.6	84
156	Phase behavior of colloidal hard perfect tetragonal parallelepipeds. *Journal of Chemical Physics*, **2008**, 128, 044909	3.9	83
155	Simulation and prediction of vapour-liquid equilibria for chain molecules. *Molecular Physics*, **1996**, 87, 347-366	1.7	77
154	Simulation of the gyroid phase in off-lattice models of pure diblock copolymer melts. *Journal of Chemical Physics*, **2006**, 125, 104907	3.9	74
153	Reaction coordinates and transition pathways of rare events via forward flux sampling. *Journal of Chemical Physics*, **2007**, 127, 164101	3.9	69
152	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, 3412-9	4	68
151	Molecular simulation of polymeric networks and gels: phase behavior and swelling. *Physics Reports*, **1999**, 318, 85-112	27.7	65
150	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	11.5	64
149	Phase behavior of colloidal hard tetragonal parallelepipeds (cuboids): a Monte Carlo simulation study. *Journal of Physical Chemistry B*, **2005**, 109, 23008-15	3.4	64
148	Monte Carlo simulation of branched and crosslinked polymers. *Journal of Chemical Physics*, **1996**, 104, 4788-4801	3.9	63
147	Molecular dynamics simulation of the mesophase behaviour of a model bolaamphiphilic liquid crystal with a lateral flexible chain. *Soft Matter*, **2008**, 4, 1820	3.6	62

146	Novel pseudoensembles for simulation of multicomponent phase equilibria. *Journal of Chemical Physics*, **1998**, 108, 8761-8772	3.9	62
145	Monte Carlo simulation of athermal mesogenic chains: Pure systems, mixtures, and constrained environments. *Journal of Chemical Physics*, **1997**, 106, 9858-9868	3.9	61
144	Cubatic liquid-crystalline behavior in a system of hard cuboids. *Journal of Chemical Physics*, **2004**, 120, 9383-9	3.9	60
143	Simulation study of free-energy barriers in the wetting transition of an oily fluid on a rough surface with reentrant geometry. *Langmuir*, **2012**, 28, 16080-90	4	59
142	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	9.6	58
141	Structure and transport properties of polymer grafted nanoparticles. *Journal of Chemical Physics*, **2011**, 135, 184902	3.9	57
140	Lattice Monte Carlo Simulations of the Gyroid Phase in Monodisperse and Bidisperse Block Copolymer Systems. *Macromolecules*, **2005**, 38, 8522-8531	5.5	56
139	Thermodynamics and kinetics of bubble nucleation: simulation methodology. *Journal of Chemical Physics*, **2012**, 137, 074109	3.9	55
138	Simulation and theory of the swelling of athermal gels. *Journal of Chemical Physics*, **1997**, 106, 793-810	3.9	55
137	Molecular dynamics of equilibrium and pressure-driven transport properties of water through LTA-type zeolites. *Langmuir*, **2013**, 29, 12389-99	4	54
136	Transition path sampling and forward flux sampling. Applications to biological systems. *Journal of Physics Condensed Matter*, **2009**, 21, 333101	1.8	53
135	A configurational-bias approach for the simulation of inner sections of linear and cyclic molecules. *Journal of Chemical Physics*, **2000**, 113, 11382-11392	3.9	50
134	Synthesis and assembly of nonspherical hollow silica colloids under confinement. *Journal of Materials Chemistry*, **2008**, 18, 4912		49
133	Optimizing the sampling and staging for simulations of rare events via forward flux sampling schemes. *Journal of Chemical Physics*, **2008**, 129, 024115	3.9	49
132	Optimization of expanded ensemble methods. *Journal of Chemical Physics*, **2008**, 129, 154107	3.9	49
131	On the use of Bennett's acceptance ratio method in multi-canonical-type simulations. *Journal of Chemical Physics*, **2004**, 120, 3066-74	3.9	47
130	Expanded ensemble and replica exchange methods for simulation of protein-like systems. *Journal of Chemical Physics*, **2003**, 119, 11998-12010	3.9	45
129	Bicontinuous Phases in Diblock Copolymer/Homopolymer Blends: Simulation and Self-Consistent Field Theory. *Macromolecules*, **2009**, 42, 1775-1784	5.5	43

128	Molecular simulations in chemical engineering: Present and future. *AICHE Journal*, **2002**, 48, 2716-2721	3.6	43
127	Simulation of Vapor□liquid Equilibria for Alkane Mixtures. *Industrial & Engineering Chemistry Research*, **1998**, 37, 3195-3202	3.9	43
126	Single polymer growth dynamics. *Science*, **2017**, 358, 352-355	33.3	42
125	Optimized expanded ensembles for simulations involving molecular insertions and deletions. I. Closed systems. *Journal of Chemical Physics*, **2007**, 127, 174103	3.9	42
124	Effect of shear on nanoparticle dispersion in polymer melts: A coarse-grained molecular dynamics study. *Journal of Chemical Physics*, **2010**, 132, 024901	3.9	41
123	Chemical potential and equations of state of hard core chain molecules. *Journal of Chemical Physics*, **1995**, 103, 1946-1956	3.9	41
122	Characterizing the structural behavior of selected A╪42 monomers with different solubilities. *Journal of Physical Chemistry B*, **2011**, 115, 4900-10	3.4	40
121	Engineering entropy in soft matter: the bad, the ugly and the good. *Soft Matter*, **2014**, 10, 8388-400	3.6	38
120	Simulation of Isoenthalps and Joule-Thomson Inversion Curves of Pure Fluids and Mixtures. *Molecular Simulation*, **2001**, 26, 395-416	2	37
119	Monte Carlo Simulation of the Effect of Entanglements on the Swelling and Deformation Behavior of End-Linked Polymeric Networks. *Macromolecules*, **2002**, 35, 3296-3305	5.5	37
118	Experiments and Simulations: Enhanced Mechanical Properties of End-Linked Bimodal Elastomers. *Macromolecules*, **2008**, 41, 8231-8241	5.5	36
117	Monte Carlo Study of the Stabilization of Complex Bicontinuous Phases in Diblock Copolymer Systems. *Macromolecules*, **2007**, 40, 7354-7365	5.5	36
116	Glassy dislocation dynamics in 2D colloidal dimer crystals. *Physical Review Letters*, **2010**, 105, 078301	7.4	34
115	Rotator and crystalline films viaself-assembly of short-bond-length colloidal dimers. *Journal of Materials Chemistry*, **2009**, 19, 344-349		33
114	Coarse-grained molecular dynamics simulation on the placement of nanoparticles within symmetric diblock copolymers under shear flow. *Journal of Chemical Physics*, **2008**, 128, 164909	3.9	33
113	Tracing coexistence lines in multicomponent fluid mixtures by molecular simulation. *Journal of Chemical Physics*, **1999**, 110, 11999-12010	3.9	32
112	The Plumber□ Nightmare Phase in Diblock Copolymer/Homopolymer Blends. A Self-Consistent Field Theory Study.. *Macromolecules*, **2009**, 42, 9058-9062	5.5	30
111	A general framework for non-Boltzmann Monte Carlo sampling. *Journal of Chemical Physics*, **2006**, 124, 054116	3.9	30

110	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	3.9	29
109	Pseudo-ensemble simulations and GibbsDuhem integrations for polymers. *Journal of Chemical Physics*, **1997**, 106, 2911-2923	3.9	28
108	Monte Carlo simulation of polymer chain collapse in an athermal solvent. *Journal of Chemical Physics*, **1997**, 106, 1288-1290	3.9	28
107	On the use of transition matrix methods with extended ensembles. *Journal of Chemical Physics*, **2006**, 124, 104110	3.9	28
106	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	7.6	27
105	Chemical potential and dimensions of chain molecules in athermal environments. *Molecular Physics*, **1996**, 89, 1733-1754	1.7	27
104	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, 9699-703	11.5	26
103	Localized orientational order chaperones the nucleation of rotator phases in hard polyhedral particles. *Physical Review Letters*, **2014**, 112, 048301	7.4	26
102	Mesoscopic structure prediction of nanoparticle assembly and coassembly: theoretical foundation. *Journal of Chemical Physics*, **2010**, 133, 194108	3.9	26
101	Simulation of bulk, confined, and polydisperse systems. I. A unified methodological framework. *Journal of Chemical Physics*, **2001**, 115, 5642-5652	3.9	26
100	Effect of quenched size polydispersity on the ordering transitions of hard polyhedral particles. *Journal of Chemical Physics*, **2012**, 137, 024905	3.9	25
99	Optimized expanded ensembles for simulations involving molecular insertions and deletions. II. Open systems. *Journal of Chemical Physics*, **2007**, 127, 174104	3.9	24
98	Predicting chiral nanostructures, lattices and superlattices in complex multicomponent nanoparticle self-assembly. *Nano Letters*, **2012**, 12, 3218-23	11.5	23
97	Folding kinetics of a lattice protein via a forward flux sampling approach. *Journal of Chemical Physics*, **2006**, 125, 164904	3.9	23
96	Phase behavior of binary mixtures of hard convex polyhedra. *Soft Matter*, **2013**, 9, 11557	3.6	22
95	Self-assembly of binary space-tessellating compounds. *Journal of Chemical Physics*, **2012**, 137, 194907	3.9	22
94	Computational affinity maturation of camelid single-domain intrabodies against the nonamyloid component of alpha-synuclein. *Scientific Reports*, **2018**, 8, 17611	4.9	22
93	Phase behavior of polyhedral nanoparticles in parallel plate confinement. *Soft Matter*, **2016**, 12, 1506-16	3.6	21

92	Directed self-assembly of spherical caps via confinement. *Soft Matter*, **2013**, 9, 9153	3.6	21
91	Protein translocation through a tunnel induces changes in folding kinetics: a lattice model study. *Biotechnology and Bioengineering*, **2006**, 94, 105-17	4.9	21
90	Liquid crystalline behavior of a semifluorinated oligomer. *Journal of Chemical Physics*, **2004**, 121, 11463-73	3.9	21
89	Hybrid Monte Carlo with multidimensional replica exchanges: conformational equilibria of the hypervariable regions of a llama VHH antibody domain. *Biopolymers*, **2003**, 68, 160-77	2.2	21
88	Simulating the kinetics and thermodynamics of transitions via forward flux/umbrella sampling. *Journal of Physical Chemistry B*, **2009**, 113, 6434-45	3.4	20
87	Variance minimization of free energy estimates from optimized expanded ensembles. *Journal of Physical Chemistry B*, **2008**, 112, 8120-8	3.4	20
86	Multicanonical schemes for mapping out free-energy landscapes of single-component and multicomponent systems. *Journal of Chemical Physics*, **2005**, 122, 164103	3.9	20
85	Simulation and extrapolation of coexistence properties with single-phase and two-phase ensembles. *Journal of Chemical Physics*, **2000**, 113, 8444-8456	3.9	20
84	Computation of Free Energies of Cubic Bicontinuous Phases for Blends of Diblock Copolymer and Selective Homopolymer. *Macromolecules*, **2016**, 49, 5232-5243	5.5	20
83	Influence of polymer architecture and polymer-wall interaction on the adsorption of polymers into a slit-pore. *Physical Review E*, **2004**, 69, 021802	2.4	19
82	Conformational Properties and Entropic Partitioning of Topologically Complex Polymers under Confinement. *Macromolecules*, **2001**, 34, 8802-8810	5.5	19
81	Simulation of swelling of model polymeric gels by subcritical and supercritical solvents. *Journal of Chemical Physics*, **1999**, 110, 1290-1298	3.9	19
80	Simulation of Chain-length Partitioning in a Microfabricated Channel via Entropic Trapping. *Molecular Simulation*, **2003**, 29, 417-425	2	18
79	A new method for generating volume changes in isobaric-isothermal Monte Carlo simulations of flexible molecules. *Macromolecular Theory and Simulations*, **1995**, 4, 691-707	1.5	18
78	Correlation between Ionic Mobility and Microstructure in Block Copolymers. A Coarse-Grained Modeling Study. *Macromolecules*, **2018**, 51, 9213-9221	5.5	18
77	Structure Control of a π-Conjugated Oligothiophene-Based Liquid Crystal for Enhanced Mixed Ion/Electron Transport Characteristics. *ACS Nano*, **2019**, 13, 7665-7675	16.7	17
76	Far-from-equilibrium sheared colloidal liquids: disentangling relaxation, advection, and shear-induced diffusion. *Physical Review E*, **2013**, 88, 062309	2.4	17
75	A novel algorithm for characterization of order in materials. *Journal of Chemical Physics*, **2002**, 117, 4000-4009	3.9	17

74	Mechanical Properties of Tetrapolyethylene and Tetrapoly(ethylene oxide) Diamond Networks via Molecular Dynamics Simulations. *Macromolecules*, **2016**, 49, 2375-2386	5.5	16
73	Entropic self-assembly of freely rotating polyhedral particles confined to a flat interface. *Soft Matter*, **2015**, 11, 1481-91	3.6	16
72	Mapping coexistence lines via free-energy extrapolation: application to order-disorder phase transitions of hard-core mixtures. *Journal of Chemical Physics*, **2014**, 140, 094102	3.9	16
71	A Novel Configurational-Bias Monte Carlo Method for Lattice Polymers: Application to Molecules with Multicyclic Architectures. *Macromolecules*, **2005**, 38, 8532-8545	5.5	16
70	Complex Relationship between Side-Chain Polarity, Conductivity, and Thermal Stability in Molecularly Doped Conjugated Polymers. *Chemistry of Materials*, **2021**, 33, 741-753	9.6	16
69	Molecular dynamics simulation of thermotropic bolaamphiphiles with a swallow-tail lateral chain: formation of cubic network phases. *Soft Matter*, **2017**, 13, 8542-8555	3.6	15
68	Sawtooth Tensile Response of Model Semiflexible and Block Copolymer Elastomers. *Macromolecules*, **2014**, 47, 840-850	5.5	15
67	Simultaneous estimation of free energies and rates using forward flux sampling and mean first passage times. *Journal of Chemical Physics*, **2015**, 143, 244113	3.9	15
66	A theoretical and simulation study of the self-assembly of a binary blend of diblock copolymers. *Journal of Chemical Physics*, **2012**, 136, 234905	3.9	15
65	Diffusivities and Viscosities of Poly(ethylene oxide) Oligomers *Journal of Chemical & Engineering Data*, **2010**, 55, 4273-4280	2.8	15
64	A unified methodological framework for the simulation of nonisothermal ensembles. *Journal of Chemical Physics*, **2005**, 123, 044110	3.9	15
63	Self-Assembly Behavior of an Oligothiophene-Based Conjugated Liquid Crystal and Its Implication for Ionic Conductivity Characteristics. *Advanced Functional Materials*, **2019**, 29, 1805220	15.6	15
62	Formation and Characterization of Semiflexible Polymer Networks via Monte Carlo Simulations. *Macromolecules*, **2004**, 37, 3924-3933	5.5	14
61	On the Scaling of the Critical Solution Temperature of Binary Polymer Blends with Chain Length. *Macromolecules*, **1999**, 32, 900-910	5.5	14
60	Heuristic rule for binary superlattice coassembly: mixed plastic mesophases of hard polyhedral nanoparticles. *Physical Review Letters*, **2014**, 113, 165504	7.4	13
59	A simulation study of lyotropic isotropic ematic phase transitions in polydisperse chain systems. *Journal of Chemical Physics*, **2003**, 118, 10262-10275	3.9	13
58	Molecular and macroscopic modeling of phase separation. *AICHE Journal*, **2000**, 46, 2086-2096	3.6	13
57	Simulation of bulk, confined, and polydisperse systems. II. Application to chain systems. *Journal of Chemical Physics*, **2001**, 115, 5653-5661	3.9	13

56	STUDY OF SOLID-LIQUID EXTRACTIONS IN A BATCH EQUIPMENT. *Chemical Engineering Communications*, **1998**, 167, 73-86	2.2	13
55	Degenerate crystals from colloidal dimers under confinement. *Soft Matter*, **2014**, 10, 9729-38	3.6	12
54	2H NMR and Simulation Studies of Chain Segment Orientation in PDMS Bimodal Networks. *Macromolecules*, **2010**, 43, 7173-7184	5.5	12
53	Simulation and prediction of vapour-liquid equilibria for chain molecules		11
52	Optimizing the formation of colloidal compounds with components of different shapes. *Journal of Chemical Physics*, **2017**, 147, 214501	3.9	10
51	Extensions of the interfacial pinning method and application to hard core systems. *Journal of Chemical Physics*, **2014**, 141, 124117	3.9	10
50	Simulation of the density of states in isothermal and adiabatic ensembles. *Physical Review E*, **2006**, 73, 056701	2.4	10
49	Nucleus-size pinning for determination of nucleation free-energy barriers and nucleus geometry. *Journal of Chemical Physics*, **2018**, 148, 184104	3.9	10
48	Stepwise elastic behavior in a model elastomer. *Physical Review Letters*, **2004**, 93, 257804	7.4	9
47	On the application of virtual Gibbs ensembles to the direct simulation of fluidfluid and solidfluid phase coexistence. *Journal of Chemical Physics*, **2002**, 116, 7957-7966	3.9	9
46	Developing Local Order Parameters for OrderDisorder Transitions From Particles to Block Copolymers: Methodological Framework. *Macromolecules*, **2018**, 51, 9769-9780	5.5	9
45	Tuning the Sawtooth Tensile Response and Toughness of Multiblock Copolymer Diamond Networks. *Macromolecules*, **2016**, 49, 6711-6721	5.5	8
44	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	3.4	8
43	Monte Carlo Simulation of the Topology and Conformational Behavior of Hyperbranched Molecules: PdDiimine-Catalyzed Polyethylene. *Macromolecular Theory and Simulations*, **2002**, 11, 136-146	1.5	8
42	Developing Local Order Parameters for OrderDisorder Transitions From Particles to Block Copolymers: Application to Macromolecular Systems. *Macromolecules*, **2018**, 51, 9781-9788	5.5	8
41	Transport Properties of Amine/Carbon Dioxide Reactive Mixtures and Implications to Carbon Capture Technologies. *ACS Applied Materials & Interfaces*, **2015**, 7, 17603-13	9.5	7
40	Solid-phase nucleation free-energy barriers in truncated cubes: interplay of localized orientational order and facet alignment. *Soft Matter*, **2018**, 14, 1996-2005	3.6	7
39	Kinetics and reaction coordinates of the reassembly of protein fragments via forward flux sampling. *Biophysical Journal*, **2010**, 98, 1911-20	2.9	7

38	In silico protein fragmentation reveals the importance of critical nuclei on domain reassembly. *Biophysical Journal*, **2008**, 94, 1575-88	2.9	7
37	Bridging continuum and statistical thermodynamics via equations of state and the density of states. *Journal of Chemical Physics*, **2004**, 120, 10699-710	3.9	7
36	Phase behaviour of model polymeric networks and gels. *Molecular Physics*, **1997**, 90, 437-443	1.7	7
35	Correlation between morphology and anisotropic transport properties of diblock copolymers melts. *Soft Matter*, **2019**, 15, 851-859	3.6	6
34	Extraction of Segment Orientation Distributions in Polymer Networks by Inversion of 2H NMR Spectra through the Maximum-Entropy Method. *Macromolecules*, **2009**, 42, 8889-8898	5.5	6
33	Creating microenvironments using encapsulated polymers. *Journal of Polymer Science Part A*, **2008**, 46, 2309-2315	2.5	6
32	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	3.9	6
31	Side chain engineering control of mixed conduction in oligoethylene glycol-substituted polythiophenes. *Journal of Materials Chemistry A*, **2021**, 9, 21410-21423	13	6
30	Optimizing the formation of solid solutions with components of different shapes. *Journal of Chemical Physics*, **2017**, 146, 134508	3.9	5
29	Exploration of factors affecting the onset and maturation course of follicular lymphoma through simulations of the germinal center. *Bulletin of Mathematical Biology*, **2009**, 71, 1432-62	2.1	5
28	Simulated mutagenesis of the hypervariable loops of a llama VHH domain for the recovery of canonical conformations. *Journal of Physical Chemistry B*, **2009**, 113, 1785-95	3.4	5
27	Gibbs-Duhem integration in lattice systems. *Europhysics Letters*, **1997**, 40, 111-116	1.6	5
26	Optimizing the network topology of block copolymer liquid crystal elastomers for enhanced extensibility and toughness. *Physical Review Materials*, **2017**, 1,	3.2	5
25	Monte Carlo Methods for Polymeric Systems. *Advances in Chemical Physics*,337-367		5
24	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	4.2	4
23	Phase behaviour of PMMA-b-PHEMA with solvents methanol and THF: modelling and comparison to the experiment. *Soft Matter*, **2014**, 10, 6172-81	3.6	4
22	Yielding and shear induced melting of 2D mixed crystals of spheres and dimers. *Soft Matter*, **2012**, 8, 5916	3.6	4
21	Reaction Fronts in a Porous Medium. Approximation Techniques versus Numerical Solution. *Industrial & Engineering Chemistry Research*, **1995**, 34, 794-805	3.9	4

20	Modeling the orientational and positional behavior of polyhedral nanoparticles at fluid-fluid interfaces. *Physical Review Materials*, **2017**, 1,	3.2	4
19	Disorder Foreshadows Order in Colloidal Cubes. *Journal of Physical Chemistry B*, **2018**, 122, 9264-9273	3.4	4
18	Swelling and Tensile Properties of Tetra-Polyethylene glycol via Coarse-Grained Molecular Models. *Macromolecular Theory and Simulations*, **2017**, 26, 1600098	1.5	3
17	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	6.4	3
16	Stability of the Gyroid Phase in Rod-Coil Systems via Thermodynamic Integration with Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 5984-5991	6.4	3
15	Thermal Stability of Conjugated n-Ethylene-Glycol-Terminated Quaterthiophene Oligomers: A Computational and Experimental Study. *ACS Macro Letters*, **2020**, 9, 295-300	6.6	2
14	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, 233-41	9.3	2
13	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
12	Simulation of chain molecules for prediction of thermodynamic properties. *Fluid Phase Equilibria*, **1996**, 116, 312-319	2.5	2
11	Framework for Inverse Mapping Chemistry-Agnostic Coarse-Grained Simulation Models into Chemistry-Specific Models. *Journal of Chemical Information and Modeling*, **2019**, 59, 5045-5056	6.1	2
10	Molecular Simulations of Laser Spike Annealing of Block Copolymer Lamellar Thin-Films. *Langmuir*, **2020**, 36, 5754-5764	4	1
9	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	5.5	1
8	Bridging hexatic and tetratic phases in binary mixtures through near critical point fluctuations. *Physical Review Materials*, **2021**, 5,	3.2	1
7	Heat capacities of supercritical fluids via Grand Canonical ensemble simulations. *Molecular Simulation*, **2018**, 44, 147-155	2	1
6	Effect of Block Immiscibility on Strain-Induced Microphase Segregation and Crystallization of Model Block Copolymer Elastomers. *Macromolecules*, **2018**, 51, 5685-5693	5.5	0
5	Computing free energy barriers for the nucleation of complex network mesophases.. *Journal of Chemical Physics*, **2022**, 156, 034502	3.9	0
4	Congruent phase behavior of a binary compound crystal of colloidal spheres and dimpled cubes. *Journal of Chemical Physics*, **2020**, 153, 214503	3.9	0
3	Low Interfacial Free Energy Describes the Bulk Ordering Transition in Colloidal Cubes. *Journal of Physical Chemistry B*, **2021**, 125, 5160-5170	3.4	0

2	On the calculation of free energies over Hamiltonian and order parameters via perturbation and thermodynamic integration. *Journal of Chemical Physics*, **2021**, 155, 114112	3.9	0
1	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	9.3	0