Athanassios Panagiotopoulos

List of Publications by Year in Descending Order

327 papers	17,792 citations	63 h-index	120 g-index
347 ext. papers	19,090 ext. citations	4.5 avg, IF	7.1 L-index

#	Paper	IF	Citations
327	Dissolving salt is not equivalent to applying a pressure on water.. *Nature Communications*, **2022**, 13, 822	17.4	10
326	A deep potential model with long-range electrostatic interactions.. *Journal of Chemical Physics*, **2022**, 156, 124107	3.9	7
325	Transferability of data-driven, many-body models for CO simulations in the vapor and liquid phases.. *Journal of Chemical Physics*, **2022**, 156, 104503	3.9	3
324	Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model.. *Journal of Physical Chemistry Letters*, **2022**, 3652-3658	6.4	4
323	Activity coefficients of aqueous electrolytes from implicit-water molecular dynamics simulations. *Journal of Chemical Physics*, **2021**, 155, 184501	3.9	0
322	Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional. *Journal of Chemical Theory and Computation*, **2021**, 17, 3065-3077	6.4	14
321	Vapor-liquid equilibrium of water with the MB-pol many-body potential. *Journal of Chemical Physics* , **2021**, 154, 211103	3.9	11
320	Individual Ion Activity Coefficients in Aqueous Electrolytes from Explicit-Water Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 8511-8521	3.4	3
319	Predicting chemical reaction equilibria in molten carbonate fuel cells via molecular simulations. *AICHE Journal*, **2021**, 67, e16988	3.6	4
318	When do short-range atomistic machine-learning models fall short?. *Journal of Chemical Physics*, **2021**, 154, 034111	3.9	26
317	First-Principles Modeling of Transport Mechanisms in Carbonate□Hydroxide Electrolytes. *Journal of Physical Chemistry C*, **2021**, 125, 4412-4422	3.8	0
316	Phase separation vs aggregation behavior for model disordered proteins. *Journal of Chemical Physics*, **2021**, 155, 125101	3.9	11
315	Shear-induced ordering in systems with competing interactions: A machine learning study. *Journal of Chemical Physics*, **2020**, 152, 204905	3.9	5
314	Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions. *Journal of Chemical Physics*, **2020**, 153, 010903	3.9	16
313	Model for disordered proteins with strongly sequence-dependent liquid phase behavior. *Journal of Chemical Physics*, **2020**, 152, 075101	3.9	54
312	Activity Coefficients and Solubility of CaCl2 from Molecular Simulations. *Journal of Chemical & Engineering Data*, **2020**, 65, 337-348	2.8	9
311	Transport and Interfacial Properties of Mixed Molten Carbonate/Hydroxide Electrolytes by Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2020**, 124, 23532-23540	3.8	3

310	Signatures of a liquid-liquid transition in an ab initio deep neural network model for water. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 26040-26046	11.5	45
309	Molecular simulation of liquid-vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models. *Journal of Chemical Physics*, **2020**, 153, 024501	3.9	7
308	Genetic Algorithm Driven Force Field Parameterization for Molten Alkali-Metal Carbonate and Hydroxide Salts. *Journal of Chemical Theory and Computation*, **2020**, 16, 5736-5746	6.4	8
307	Thermodynamic analysis of the stability of planar interfaces between coexisting phases and its application to supercooled water. *Journal of Chemical Physics*, **2019**, 150, 224503	3.9	4
306	Self-Organization and Flow of Low-Functionality Telechelic Star Polymers with Varying Attraction. *ACS Macro Letters*, **2019**, 8, 766-772	6.6	12
305	Quantized bounding volume hierarchies for neighbor search in molecular simulations on graphics processing units. *Computational Materials Science*, **2019**, 164, 139-146	3.2	5
304	Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal. *Journal of Chemical Physics*, **2019**, 150, 124502	3.9	42
303	Dynamic properties of aqueous electrolyte solutions from non-polarisable, polarisable, and scaled-charge models. *Molecular Physics*, **2019**, 117, 3538-3549	1.7	17
302	Unexpected secondary flows in reverse nonequilibrium shear flow simulations. *Physical Review Fluids*, **2019**, 4,	2.8	6
301	Self-Assembly of Polymer Blends and Nanoparticles through Rapid Solvent Exchange. *Langmuir*, **2019**, 35, 3780-3789	4	4
300	On the Stability of Polymeric Nanoparticles Fabricated through Rapid Solvent Mixing. *Langmuir*, **2019**, 35, 709-717	4	16
299	Directed assembly of photonic crystals through simple substrate patterning. *Journal of Chemical Physics*, **2019**, 150, 014503	3.9	5
298	Molecular Modeling of Surfactant Micellization Using Solvent-Accessible Surface Area. *Langmuir*, **2019**, 35, 2443-2450	4	22
297	Crystal growth kinetics of triblock Janus colloids. *Journal of Chemical Physics*, **2018**, 148, 124506	3.9	13
296	Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions. *Journal of Chemical Physics*, **2018**, 148, 044505	3.9	30
295	Comment on "The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water" [I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]. *Journal of Chemical Physics*, **2018**, 148, 137101	3.9	50
294	Communication: Modeling electrolyte mixtures with concentration dependent dielectric permittivity. *Journal of Chemical Physics*, **2018**, 148, 041102	3.9	4
293	System-Size Dependence of Electrolyte Activity Coefficients in Molecular Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 3330-3338	3.4	12

292	Rapid Production of Internally Structured Colloids by Flash Nanoprecipitation of Block Copolymer Blends. *ACS Nano*, **2018**, 12, 4660-4668	16.7	49
291	Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration. *Computer Physics Communications*, **2018**, 230, 10-20	4.2	30
290	Influence of hydrodynamic interactions on stratification in drying mixtures. *Journal of Chemical Physics*, **2018**, 149, 024902	3.9	21
289	Automated crystal characterization with a fast neighborhood graph analysis method. *Soft Matter*, **2018**, 14, 6083-6089	3.6	22
288	Preface: Special Topic on Enhanced Sampling for Molecular Systems. *Journal of Chemical Physics*, **2018**, 149, 072001	3.9	2
287	Differences in free surfactant concentration and aggregation properties for amphiphiles with the same critical micelle concentration. *Fluid Phase Equilibria*, **2018**, 470, 126-133	2.5	15
286	Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field. *Journal of Chemical Physics*, **2018**, 149, 141102	3.9	14
285	Evaporation-induced assembly of colloidal crystals. *Journal of Chemical Physics*, **2018**, 149, 094901	3.9	18
284	Multi-scale simulations of polymeric nanoparticle aggregation during rapid solvent exchange. *Journal of Chemical Physics*, **2018**, 149, 084904	3.9	5
283	Phase Equilibria of Water/CO and Water/n-Alkane Mixtures from Polarizable Models. *Journal of Physical Chemistry B*, **2017**, 121, 1386-1395	3.4	21
282	Molecular Modeling of Thermodynamic and Transport Properties for CO and Aqueous Brines. *Accounts of Chemical Research*, **2017**, 50, 751-758	24.3	16
281	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. *Physical Review B*, **2017**, 95,	3.3	12
280	Directionally Interacting Spheres and Rods Form Ordered Phases. *ACS Nano*, **2017**, 11, 4950-4959	16.7	17
279	Machine learning for autonomous crystal structure identification. *Soft Matter*, **2017**, 13, 4733-4745	3.6	64
278	Stratification Dynamics in Drying Colloidal Mixtures. *Langmuir*, **2017**, 33, 3685-3693	4	56
277	Structured Nanoparticles from the Self-Assembly of Polymer Blends through Rapid Solvent Exchange. *Langmuir*, **2017**, 33, 6021-6028	4	24
276	Vapour–liquid phase equilibrium and surface tension of fully flexible Lennard–Jones chains. *Molecular Physics*, **2017**, 115, 320-327	1.7	52
275	Thermodynamic signatures and cluster properties of self-assembly in systems with competing interactions. *Soft Matter*, **2017**, 13, 8055-8063	3.6	22

274	Controlled production of patchy particles from the combined effects of nanoprecipitation and vitrification. *Soft Matter*, **2017**, 13, 8433-8441	3.6	15
273	Contact angles from Young's equation in molecular dynamics simulations. *Journal of Chemical Physics*, **2017**, 147, 084708	3.9	36
272	Multi-atom pattern analysis for binary superlattices. *Soft Matter*, **2017**, 13, 6803-6809	3.6	11
271	Characterization of the liquid Li-solid Mo (1 1 0) interface from classical molecular dynamics for plasma-facing applications. *Nuclear Fusion*, **2017**, 57, 116036	3.3	4
270	Stratification in Drying Polymer-Polymer and Colloid-Polymer Mixtures. *Langmuir*, **2017**, 33, 11390-11398	4	42
269	Polymer Chain Collapse upon Rapid Solvent Exchange: Slip-Spring Dissipative Particle Dynamics Simulations with an Explicit-Solvent Model. *Journal of Physical Chemistry C*, **2017**, 121, 27664-27673	3.8	7
268	Solvent quality influences surface structure of glassy polymer thin films after evaporation. *Journal of Chemical Physics*, **2017**, 147, 184901	3.9	6
267	Note: Smooth torsional potentials for degenerate dihedral angles. *Journal of Chemical Physics*, **2017**, 146, 226101	3.9	6
266	Self-diffusion coefficients of the binary (H 2 O + CO 2) mixture at high temperatures and pressures. *Journal of Chemical Thermodynamics*, **2016**, 93, 424-429	2.9	30
265	Hydration Repulsion between Carbohydrate Surfaces Mediated by Temperature and Specific Ions. *Scientific Reports*, **2016**, 6, 28553	4.9	17
264	Porphyrin-Sensitized Evolution of Hydrogen using Dawson and Keplerate Polyoxometalate Photocatalysts. *ChemSusChem*, **2016**, 9, 3213-3219	8.3	23
263	Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. *Journal of Physical Chemistry B*, **2016**, 120, 12358-12370	3.4	28
262	Monte Carlo simulations of H2O□aCl2 and H2O□aCl2□O2 mixtures. *Fluid Phase Equilibria*, **2016**, 407, 262-268	2.5	11
261	Gaussian-Charge Polarizable and Nonpolarizable Models for CO2. *Journal of Physical Chemistry B*, **2016**, 120, 984-94	3.4	25
260	Palmer et al. reply. *Nature*, **2016**, 531, E2-3	50.4	14
259	Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units. *Computer Physics Communications*, **2016**, 203, 45-52	4.2	35
258	Modeling of CO2 solubility in single and mixed electrolyte solutions using statistical associating fluid theory. *Geochimica Et Cosmochimica Acta*, **2016**, 176, 185-197	5.5	14
257	Directed Assembly of Soft Colloids through Rapid Solvent Exchange. *ACS Nano*, **2016**, 10, 1425-33	16.7	49

256	Axial dispersion of Brownian colloids in microfluidic channels. *Physical Review Fluids*, **2016**, 1,	2.8	10
255	Void-Based Assembly of Colloidal Crystals: Using Structure-Directing Agents to Direct the Assembly of Open Colloidal Crystals **2016**, 5, 1-5		
254	Water: A Tale of Two Liquids. *Chemical Reviews*, **2016**, 116, 7463-500	68.1	453
253	Equilibrium crystal phases of triblock Janus colloids. *Journal of Chemical Physics*, **2016**, 145, 094505	3.9	26
252	Atomistic Molecular Dynamics Simulations of Carbon Dioxide Diffusivity in n-Hexane, n-Decane, n-Hexadecane, Cyclohexane, and Squalane. *Journal of Physical Chemistry B*, **2016**, 120, 12890-12900	3.4	39
251	On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures. *Journal of Chemical Physics*, **2016**, 145, 154111	3.9	60
250	Determination of the critical micelle concentration in simulations of surfactant systems. *Journal of Chemical Physics*, **2016**, 144, 044709	3.9	36
249	Note: Activity coefficients and solubilities for the NaCl/? force field. *Journal of Chemical Physics*, **2016**, 145, 046101	3.9	10
248	Force Fields for Carbohydrate-Divalent Cation Interactions. *Journal of Physical Chemistry B*, **2016**, 120, 5203-8	3.4	9
247	Photochemical hydrogen production and cobaloximes: the influence of the cobalt axial N-ligand on the system stability. *Dalton Transactions*, **2016**, 45, 6732-8	4.3	59
246	Bottom-Up Colloidal Crystal Assembly with a Twist. *ACS Nano*, **2016**, 10, 5459-67	16.7	28
245	Self-assembly of Janus particles under shear. *Soft Matter*, **2015**, 11, 3767-71	3.6	31
244	Thermodynamic and Transport Properties of H2O + NaCl from Polarizable Force Fields. *Journal of Chemical Theory and Computation*, **2015**, 11, 3802-10	6.4	49
243	Customizing wormlike mesoscale structures via self-assembly of amphiphilic star polymers. *Soft Matter*, **2015**, 11, 3530-5	3.6	19
242	Atomistic molecular dynamics simulations of H2O diffusivity in liquid and supercritical CO2. *Molecular Physics*, **2015**, 113, 2805-2814	1.7	27
241	Coarse-graining and phase behavior of model star polymer-colloid mixtures in solvents of varying quality. *Journal of Chemical Physics*, **2015**, 143, 243108	3.9	6
240	Tuning polymer architecture to manipulate the relative stability of different colloid crystal morphologies. *Soft Matter*, **2015**, 11, 5146-53	3.6	10
239	Inertial and viscoelastic forces on rigid colloids in microfluidic channels. *Journal of Chemical Physics*, **2015**, 142, 224908	3.9	17

238	Grafted nanoparticles as soft patchy colloids: self-assembly versus phase separation. *Journal of Chemical Physics*, **2015**, 142, 074901	3.9	17
237	Temperature-dependent solubilities and mean ionic activity coefficients of alkali halides in water from molecular dynamics simulations. *Journal of Chemical Physics*, **2015**, 143, 044505	3.9	66
236	A Comparison of the Predictive Capabilities of the Embedded-Atom Method and Modified Embedded-Atom Method Potentials for Lithium. *Journal of Physical Chemistry B*, **2015**, 119, 8960-8	3.4	22
235	Relative stability of the FCC and HCP polymorphs with interacting polymers. *Soft Matter*, **2015**, 11, 280-9	3.6	15
234	Explicit- and implicit-solvent simulations of micellization in surfactant solutions. *Langmuir*, **2015**, 31, 3283-92	4	22
233	Liquid li structure and dynamics: A comparison between OFDFT and second nearest-neighbor embedded-atom method. *AICHE Journal*, **2015**, 61, 2841-2853	3.6	19
232	Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations. *Journal of Chemical Physics*, **2015**, 142, 044507	3.9	93
231	Grand Canonical Monte Carlo Simulations Guided by an Analytic Equation of State-Transferable Anisotropic Mie Potentials for Ethers. *Journal of Physical Chemistry B*, **2015**, 119, 7087-99	3.4	30
230	Atomistic molecular dynamics simulations of carbohydrate-calcite interactions in concentrated brine. *Langmuir*, **2015**, 31, 2407-13	4	48
229	Molecular Thermodynamic Models for CO2 and Mixtures: Recent Developments and Applications for Process Design **2015**, 361-370		
228	Self-assembly of polymer-grafted nanoparticles in thin films. *Soft Matter*, **2014**, 10, 786-94	3.6	61
227	Stabilizing colloidal crystals by leveraging void distributions. *Nature Communications*, **2014**, 5, 4472	17.4	42
226	Communication: Effect of solvophobic block length on critical micelle concentration in model surfactant systems. *Journal of Chemical Physics*, **2014**, 141, 041101	3.9	6
225	Viscosity of Nafion oligomers as a function of hydration and counterion type: a molecular dynamics study. *Journal of Physical Chemistry B*, **2014**, 118, 13981-91	3.4	11
224	Atomistic molecular dynamics simulations of CO□diffusivity in H□O for a wide range of temperatures and pressures. *Journal of Physical Chemistry B*, **2014**, 118, 5532-41	3.4	63
223	Sequential Domain Realignment Driven by Conformational Asymmetry in Block Copolymer Thin Films. *Macromolecules*, **2014**, 47, 1193-1198	5.5	15
222	Thin films of homopolymers and cylinder-forming diblock copolymers under shear. *ACS Nano*, **2014**, 8, 8015-26	16.7	32
221	Optimization of intermolecular potential parameters for the CO2/H2O mixture. *Journal of Physical Chemistry B*, **2014**, 118, 11504-11	3.4	27

220	Molecular dynamics simulations of water permeation across Nafion membrane interfaces. *Journal of Physical Chemistry B*, **2014**, 118, 8798-807	3.4	23
219	Metastable liquid-liquid transition in a molecular model of water. *Nature*, **2014**, 510, 385-8	50.4	356
218	Atomistic simulation of CO2 solubility in poly(ethylene oxide) oligomers. *Molecular Physics*, **2014**, 112, 1540-1547	1.7	4
217	Flory-Huggins parameter □from binary mixtures of Lennard-Jones particles to block copolymer melts. *Journal of Chemical Physics*, **2014**, 140, 054909	3.9	56
216	Flow-induced demixing of polymer-colloid mixtures in microfluidic channels. *Journal of Chemical Physics*, **2014**, 140, 094903	3.9	13
215	Molecular simulation of thermodynamic and transport properties for the H2O+NaCl system. *Journal of Chemical Physics*, **2014**, 141, 234507	3.9	49
214	Self-Assembly of Cylinder-Forming Diblock Copolymer Thin Films. *Macromolecules*, **2013**, 46, 6651-6658	5.5	18
213	Molecular dynamics simulation of SDS and CTAB micellization and prediction of partition equilibria with COSMOmic. *Langmuir*, **2013**, 29, 11582-92	4	47
212	Simulations of vapor□liquid phase equilibrium and interfacial tension in the CO2□H2O□NaCl system. *AICHE Journal*, **2013**, 59, 3514-3522	3.6	35
211	Simulations of shear-induced morphological transitions in block copolymers. *Soft Matter*, **2013**, 9, 9960	3.6	28
210	Molecular dynamics simulations of water sorption in a perfluorosulfonic acid membrane. *Journal of Physical Chemistry B*, **2013**, 117, 12649-60	3.4	29
209	Phase behavior of rigid, amphiphilic star polymers. *Soft Matter*, **2013**, 9, 7424	3.6	10
208	Diffusivities, viscosities, and conductivities of solvent-free ionically grafted nanoparticles. *Soft Matter*, **2013**, 9, 6091	3.6	8
207	Structure of phase-separated athermal colloid-polymer systems in the protein limit. *Physical Review E*, **2013**, 87, 022309	2.4	15
206	Phase behavior of athermal colloid-star polymer mixtures. *Journal of Chemical Physics*, **2013**, 139, 024907	3.9	16
205	A computational investigation of the phase behavior and capillary sublimation of water confined between nanoscale hydrophobic plates. *Journal of Chemical Physics*, **2012**, 137, 144501	3.9	36
204	Molecular dynamics simulations of silica nanoparticles grafted with poly(ethylene oxide) oligomer chains. *Journal of Physical Chemistry B*, **2012**, 116, 2385-95	3.4	53
203	Shear-induced alignment of lamellae in thin films of diblock copolymers. *Soft Matter*, **2012**, 8, 7803	3.6	16

202	Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units. *Soft Matter*, **2012**, 8, 2385-2397	3.6	102
201	Massively parallel chemical potential calculation on graphics processing units. *Computer Physics Communications*, **2012**, 183, 2054-2062	4.2	20
200	Atomistic simulations of micellization of sodium hexyl, heptyl, octyl, and nonyl sulfates. *Journal of Physical Chemistry B*, **2012**, 116, 2430-7	3.4	68
199	Conformational transitions of weak polyacids grafted to nanoparticles. *Journal of Chemical Physics*, **2012**, 137, 144704	3.9	14
198	Liquid-liquid transition in ST2 water. *Journal of Chemical Physics*, **2012**, 137, 214505	3.9	128
197	Simulations of the structure and dynamics of nanoparticle-based ionic liquids. *Faraday Discussions*, **2012**, 154, 29-40; discussion 81-96, 465-71	3.6	22
196	Pressure and density scaling for colloid-polymer systems in the protein limit. *Physical Review E*, **2012**, 85, 051402	2.4	17
195	Sphere-to-Cylinder Transitions in Thin Films of Diblock Copolymers under Shear: The Role of Wetting Layers. *Macromolecules*, **2012**, 45, 4406-4415	5.5	20
194	Grand-canonical Monte Carlo method for Donnan equilibria. *Physical Review E*, **2012**, 86, 016703	2.4	7
193	Dynamics in coarse-grained models for oligomer-grafted silica nanoparticles. *Journal of Chemical Physics*, **2012**, 136, 204904	3.9	23
192	Dynamics of solvent-free grafted nanoparticles. *Journal of Chemical Physics*, **2012**, 136, 044902	3.9	43
191	Dissipative particle dynamics simulations of polymer-protected nanoparticle self-assembly. *Journal of Chemical Physics*, **2011**, 135, 184903	3.9	41
190	Lattice model of oligonucleotide hybridization in solution. I. Model and thermodynamics. *Journal of Chemical Physics*, **2011**, 134, 165103	3.9	17
189	Implicit-solvent models for micellization: nonionic surfactants and temperature-dependent properties. *Journal of Physical Chemistry B*, **2011**, 115, 990-1001	3.4	29
188	Structure of solvent-free grafted nanoparticles: molecular dynamics and density-functional theory. *Journal of Chemical Physics*, **2011**, 135, 114901	3.9	48
187	Monte Carlo simulations of high-pressure phase equilibria of CO2-H2O mixtures. *Journal of Physical Chemistry B*, **2011**, 115, 6629-35	3.4	37
186	Simulations of micellization of sodium hexyl sulfate. *Journal of Physical Chemistry B*, **2011**, 115, 1403-10	3.4	39
185	Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations *Industrial & Engineering Chemistry Research*, **2011**, 50, 69-77	3.9	23

184	Interactions between charged surfaces with ionizable sites. *Langmuir*, **2011**, 27, 8761-6	4	16
183	Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach. *Chemical Physics Letters*, **2011**, 509, 1-11	2.5	103
182	Self-assembly scenarios of block copolymer stars. *Molecular Physics*, **2011**, 109, 3049-3060	1.7	12
181	Structural transitions of solvent-free oligomer-grafted nanoparticles. *Physical Review Letters*, **2011**, 107, 105503	7.4	49
180	Integrating diffusion maps with umbrella sampling: application to alanine dipeptide. *Journal of Chemical Physics*, **2011**, 134, 135103	3.9	55
179	A comparison of implicit- and explicit-solvent simulations of self-assembly in block copolymer and solute systems. *Journal of Chemical Physics*, **2011**, 134, 164902	3.9	60
178	Systematic determination of order parameters for chain dynamics using diffusion maps. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 13597-602	11.5	115
177	Micellization behavior of coarse grained surfactant models. *Journal of Chemical Physics*, **2010**, 132, 114902	3.9	64
176	Diffusivities and Viscosities of Poly(ethylene oxide) Oligomers *Journal of Chemical & Engineering Data*, **2010**, 55, 4273-4280	2.8	15
175	An experimental and computational investigation of spontaneous lasso formation in microcin J25. *Biophysical Journal*, **2010**, 99, 3056-65	2.9	51
174	Phase behavior of low-functionality, telechelic star block copolymers. *Faraday Discussions*, **2010**, 144, 143-57; discussion 203-22, 467-81	3.6	13
173	Finite-size scaling study of the vapor-liquid critical properties of confined fluids: Crossover from three dimensions to two dimensions. *Journal of Chemical Physics*, **2010**, 132, 144107	3.9	25
172	Ultra thin films of diblock copolymers under shear. *Soft Matter*, **2010**, 6, 3588	3.6	19
171	Aggregation phenomena in telechelic star polymer solutions. *Physical Review E*, **2009**, 79, 010401	2.4	34
170	Micellization and phase separation in binary amphiphile mixtures. *Molecular Physics*, **2009**, 107, 2359-2366	1.7	9
169	Low-temperature fluid-phase behavior of ST2 water. *Journal of Chemical Physics*, **2009**, 131, 104508	3.9	124
168	Orientational bonding model for temperature dependent micellization and solubility of diblock surfactants. *Journal of Chemical Physics*, **2009**, 131, 114901	3.9	5
167	Phase diagrams of charged colloids from thermodynamic integration. *Journal of Physics Condensed Matter*, **2009**, 21, 465104	1.8	6

166	Anisotropic self-assembly of spherical polymer-grafted nanoparticles. *Nature Materials*, **2009**, 8, 354-9	27	820
165	Electrostatic screening and charge correlation effects in micellization of ionic surfactants. *Journal of Physical Chemistry B*, **2009**, 113, 6314-20	3.4	46
164	Modeling the anisotropic self-assembly of spherical polymer-grafted nanoparticles. *Journal of Chemical Physics*, **2009**, 131, 221102	3.9	101
163	Charge correlation effects on ionization of weak polyelectrolytes. *Journal of Physics Condensed Matter*, **2009**, 21, 424113	1.8	24
162	Solubility and molecular conformations of n-alkane chains in water. *Journal of Physical Chemistry B*, **2009**, 113, 6405-14	3.4	116
161	Protected peptide nanoparticles: experiments and brownian dynamics simulations of the energetics of assembly. *Nano Letters*, **2009**, 9, 2218-22	11.5	39
160	Structure and dynamics of surfactant and hydrocarbon aggregates on graphite: a molecular dynamics simulation study. *Journal of Physical Chemistry B*, **2008**, 112, 2915-21	3.4	41
159	Surfactant and hydrocarbon aggregates on defective graphite surface: structure and dynamics. *Journal of Physical Chemistry B*, **2008**, 112, 12954-61	3.4	28
158	Phase behavior and structure formation in linear multiblock copolymer solutions by Monte Carlo simulation. *Journal of Chemical Physics*, **2008**, 128, 164906	3.9	26
157	Simulations of phase transitions and free energies for ionic systems. *Molecular Physics*, **2008**, 106, 2039-2051	2.1	36
156	Implicit solvent models for micellization of ionic surfactants. *Journal of Physical Chemistry B*, **2008**, 112, 13783-92	3.4	51
155	Coarse-grained simulations of rapid assembly kinetics for polystyrene-b-poly(ethylene oxide) copolymers in aqueous solutions. *Journal of Physical Chemistry B*, **2008**, 112, 16357-66	3.4	39
154	Preparation of poly(ethylene glycol) protected nanoparticles with variable bioconjugate ligand density. *Biomacromolecules*, **2008**, 9, 2705-11	6.9	99
153	Composite block copolymer stabilized nanoparticles: simultaneous encapsulation of organic actives and inorganic nanostructures. *Langmuir*, **2008**, 24, 83-90	4	150
152	Monte Carlo simulations of amphiphilic nanoparticle self-assembly. *Journal of Chemical Physics*, **2008**, 129, 194706	3.9	17
151	Monte Carlo simulation and molecular theory of tethered polyelectrolytes. *Journal of Chemical Physics*, **2007**, 126, 244902	3.9	47
150	Disappearance of the gas-liquid phase transition for highly charged colloids. *Physical Review Letters* , **2007**, 98, 198301	7.4	21
149	Effective potentials for 1:1 electrolyte solutions incorporating dielectric saturation and repulsive hydration. *Journal of Chemical Physics*, **2007**, 126, 044509	3.9	61

148	Methods for Examining Phase Equilibria. *Springer Series in Chemical Physics*, **2007**, 353-387	0.3	3
147	Methods Based on Probability Distributions and Histograms. *Springer Series in Chemical Physics*, **2007**, 77-118	0.3	8
146	Phase behavior of the lattice restricted primitive model with nearest neighbor exclusion. *Journal of Chemical Physics*, **2006**, 124, 194509	3.9	4
145	Monte carlo simulations of micellization in model ionic surfactants: application to sodium dodecyl sulfate. *Langmuir*, **2006**, 22, 4076-83	4	50
144	Global phase diagram for the honeycomb potential. *Journal of Chemical Physics*, **2006**, 125, 24505	3.9	10
143	Phase Behavior of Rigid Objects on a Cubic Lattice *Industrial & Engineering Chemistry Research*, **2006**, 45, 5421-5425	3.9	2
142	Monte Carlo Simulation of the Phase Behavior of Model Dendrimers. *Macromolecules*, **2006**, 39, 6298-6305	5.5	16
141	Phase Behavior of Binary Stockmayer and Polarizable Lennard-Jones Fluid Mixtures Using Adiabatic Nuclear and Electronic Sampling. *Industrial & Engineering Chemistry Research*, **2006**, 45, 6929-6938	3.9	5
140	Effect of stiffness on the micellization behavior of model H4T4 surfactant chains. *Langmuir*, **2006**, 22, 6514-22	4	19
139	Tracing the critical loci of binary fluid mixtures using molecular simulation. *Journal of Physical Chemistry B*, **2006**, 110, 17200-6	3.4	8
138	A conformal solution theory for the energy landscape and glass transition of mixtures. *Fluid Phase Equilibria*, **2006**, 241, 147-154	2.5	16
137	Computer simulations of phase transitions of bulk and confined colloid polymer systems. *Physica A: Statistical Mechanics and Its Applications*, **2006**, 369, 275-290	3.3	23
136	Computational characterization of the sequence landscape in simple protein alphabets. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 232-43	4.2	10
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