Luis G Macdowell

List of Publications by Citations

100 papers	3,213 citations	33 h-index	53 g-index
103 ext. papers	3,512 ext. citations	4.5 avg, IF	5.33 L-index

#	Paper	IF	Citations
100	Phase diagram of water from computer simulation. *Physical Review Letters*, **2004**, 92, 255701	7.4	245
99	Femtosecond laser reshaping yields gold nanorods with ultranarrow surface plasmon resonances. *Science*, **2017**, 358, 640-644	33.3	176
98	The evaporation/condensation transition of liquid droplets. *Journal of Chemical Physics*, **2004**, 120, 5293-308	3.9	133
97	Interface and Surface Properties of Short Polymers in Solution: Monte Carlo Simulations and Self-Consistent Field Theory. *Macromolecules*, **2000**, 33, 3902-3923	5.5	127
96	Nucleation and cavitation of spherical, cylindrical, and slablike droplets and bubbles in small systems. *Journal of Chemical Physics*, **2006**, 125, 34705	3.9	116
95	Short chains at surfaces and interfaces: A quantitative comparison between density-functional theories and Monte Carlo simulations. *Journal of Chemical Physics*, **2003**, 118, 2929	3.9	96
94	Dielectric constant of ices and water: a lesson about water interactions. *Journal of Physical Chemistry A*, **2011**, 115, 5745-58	2.8	94
93	Phase behavior of n-alkanes in supercritical solution: a Monte Carlo study. *Journal of Chemical Physics*, **2004**, 121, 2169-79	3.9	88
92	Micelle-directed chiral seeded growth on anisotropic gold nanocrystals. *Science*, **2020**, 368, 1472-1477	33.3	78
91	Equation of state and critical behavior of polymer models: A quantitative comparison between Wertheim's thermodynamic perturbation theory and computer simulations. *Journal of Chemical Physics*, **2000**, 113, 419-433	3.9	72
90	Vapor-liquid interfacial properties of fully flexible Lennard-Jones chains. *Journal of Chemical Physics*, **2008**, 129, 144703	3.9	69
89	Tracing the phase diagram of the four-site water potential (TIP4P). *Journal of Chemical Physics*, **2004**, 121, 1165-6	3.9	68
88	Nano-dewetting: Interplay between van der Waals- and short-ranged interactions. *Journal of Chemical Physics*, **2001**, 115, 9960-9969	3.9	67
87	Can simple models describe the phase diagram of water?. *Journal of Physics Condensed Matter*, **2005**, 17, S3283-S3288	1.8	62
86	Polymer + Solvent Systems: Phase Diagrams, Interface Free Energies, and Nucleation. *Advances in Polymer Science*, **2005**, 1-110	1.3	61
85	Interface properties and bubble nucleation in compressible mixtures containing polymers. *Journal of Chemical Physics*, **2002**, 117, 5480-5496	3.9	60
84	Disconnecting Symmetry Breaking from Seeded Growth for the Reproducible Synthesis of High Quality Gold Nanorods. *ACS Nano*, **2019**, 13, 4424-4435	16.7	59

83	Adsorption of polymers on a brush: Tuning the order of the wetting phase transition. *Journal of Chemical Physics*, **2006**, 124, 084907	3.9	58
82	The range of meta stability of ice-water melting for two simple models of water. *Molecular Physics*, **2005**, 103, 1-5	1.7	50
81	Combinatorial entropy and phase diagram of partially ordered ice phases. *Journal of Chemical Physics*, **2004**, 121, 10145-58	3.9	50
80	Coarse-grained models for fluids and their mixtures: Comparison of Monte Carlo studies of their phase behavior with perturbation theory and experiment. *Journal of Chemical Physics*, **2009**, 130, 044101	3.9	49
79	Wetting of polymer liquids: Monte Carlo simulations and self-consistent field calculations. *Journal of Physics Condensed Matter*, **2003**, 15, R609-R653	1.8	49
78	Direct calculation of interfacial tensions from computer simulation: results for freely jointed tangent hard sphere chains. *Physical Review E*, **2007**, 75, 061609	2.4	45
77	Liquid crystal phase formation for the linear tangent hard sphere model from Monte Carlo simulations. *Journal of Chemical Physics*, **2001**, 115, 4203-4211	3.9	45
76	Efficient prediction of thermodynamic properties of quadrupolar fluids from simulation of a coarse-grained model: the case of carbon dioxide. *Journal of Chemical Physics*, **2008**, 128, 104501	3.9	44
75	Isotropic-nematic phase transition: Influence of intramolecular flexibility using a fused hard sphere model. *Physical Review E*, **2001**, 64, 011703	2.4	44
74	Extending Wertheim's perturbation theory to the solid phase: The freezing of the pearl-necklace model. *Journal of Chemical Physics*, **2001**, 114, 10411-10418	3.9	44
73	Phase diagram of water under an applied electric field. *Physical Review Letters*, **2011**, 107, 155702	7.4	41
72	Surface tension of fully flexible Lennard-Jones chains: role of long-range corrections. *Journal of Chemical Physics*, **2009**, 131, 074705	3.9	41
71	A study of the ice-water interface using the TIP4P/2005 water model. *Physical Chemistry Chemical Physics*, **2014**, 16, 22159-66	3.6	36
70	Wetting of a short chain liquid on a brush: First-order and critical wetting transitions. *Europhysics Letters*, **2001**, 55, 221-227	1.6	36
69	Disjoining pressure and the film-height-dependent surface tension of thin liquid films: new insight from capillary wave fluctuations. *Advances in Colloid and Interface Science*, **2014**, 206, 150-71	14.3	33
68	How do droplets on a surface depend on the system size?. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2002**, 206, 277-291	5.1	33
67	Critical lines and phase coexistence of polymer solutions: A quantitative comparison between Wertheim's thermodynamic perturbation theory and computer simulations. *Journal of Chemical Physics*, **2002**, 117, 6360-6371	3.9	31
66	Premelting-Induced Smoothening of the Ice-Vapor Interface. *Physical Review Letters*, **2016**, 117, 096101	7.4	29

65	Dielectric constant of ice Ih and ice V: a computer simulation study. *Journal of Physical Chemistry B*, **2010**, 114, 6089-98	3.4	29
64	Critical temperature of infinitely long chains from Wertheim's perturbation theory. *Molecular Physics*, **2000**, 98, 1295-1308	1.7	28
63	Equation of state for hard n-alkane models: Long chains. *Journal of Chemical Physics*, **1996**, 104, 701-713	3.9	26
62	Capillary fluctuations and film-height-dependent surface tension of an adsorbed liquid film. *Physical Review Letters*, **2013**, 111, 047802	7.4	25
61	Computer simulation study of the global phase behavior of linear rigid Lennard-Jones chain molecules: comparison with flexible models. *Journal of Chemical Physics*, **2004**, 120, 3957-68	3.9	25
60	Phase diagrams of hexadecane□CO2 mixtures from histogram-reweighting Monte Carlo. *Computer Physics Communications*, **2002**, 147, 378-381	4.2	24
59	Observation of autophobic dewetting on polymer brushes from computer simulation. *Journal of Physics Condensed Matter*, **2005**, 17, S3523-S3528	1.8	24
58	Phase separation kinetics in compressible polymer solutions: computer simulation of the early stages. *New Journal of Physics*, **2004**, 6, 7-7	2.9	23
57	The virial coefficients of the pearl-necklace model. *Journal of Chemical Physics*, **2000**, 113, 10398-10409	3.9	23
56	Computer simulation study of surface wave dynamics at the crystal-melt interface. *Journal of Chemical Physics*, **2014**, 141, 034701	3.9	22
55	Computer simulation of interface potentials: Towards a first principle description of complex interfaces?. *European Physical Journal: Special Topics*, **2011**, 197, 131-145	2.3	20
54	The second virial coefficient of hard alkane models. *Journal of Chemical Physics*, **1998**, 109, 5670-5680	3.9	20
53	Understanding the critical properties of chain molecules. *Molecular Physics*, **1996**, 88, 1575-1602	1.7	20
52	Vapor-liquid interfacial properties of rigid-linear Lennard-Jones chains. *Journal of Chemical Physics*, **2012**, 137, 084706	3.9	19
51	Semi-infinite boundary conditions for the simulation of interfaces: the Ar/CO2(s) model revisited. *Journal of Chemical Physics*, **2012**, 136, 104703	3.9	19
50	Formal study of nucleation as described by fluctuation theory. *Journal of Chemical Physics*, **2003**, 119, 453-463	3.9	19
49	Self-consistent field/density functional study of conformational properties of polymers at interfaces: role of intramolecular interactions. *Journal of Chemical Physics*, **2008**, 129, 104901	3.9	18
48	The effect of flexibility on the phase diagram of simple molecular models. *Physical Chemistry Chemical Physics*, **2002**, 4, 853-862	3.6	18

47	Universal scaling behaviour of surface tension of molecular chains. *Journal of Chemical Physics*, **2012**, 137, 024702	3.9	17
46	Third virial coefficients and critical properties of quadrupolar two center Lennard-Jones models. *Physical Chemistry Chemical Physics*, **2003**, 5, 2851-2857	3.6	17
45	Critical properties of molecular fluids from the virial series. *Journal of Chemical Physics*, **2003**, 119, 11367-11373	3.9	17
44	Surface phase transitions and crystal habits of ice in the atmosphere. *Science Advances*, **2020**, 6, eaay9322	14.3	16
43	Liquid–Vapor Phase Equilibria and Surface Tension of Ethane As Predicted by the TraPPE and OPLS Models. *Journal of Chemical & Engineering Data*, **2010**, 55, 5465-5470	2.8	15
42	Computer simulation of two new solid phases of water: Ice XIII and ice XIV. *Journal of Chemical Physics*, **2006**, 125, 116101	3.9	15
41	Disjoining Pressure, Healing Distance, and Film Height Dependent Surface Tension of Thin Wetting Films. *Journal of Physical Chemistry C*, **2014**, 118, 22079-22089	3.8	14
40	Vapor–liquid equilibria of linear and branched alkanes from perturbation theory. *Journal of Chemical Physics*, **1998**, 109, 5681-5690	3.9	14
39	Ice: A fruitful source of information about liquid water. *Journal of Molecular Liquids*, **2007**, 136, 214-220	6	14
38	Equation of state of model branched alkanes: Theoretical predictions and configurational bias Monte Carlo simulations. *Journal of Chemical Physics*, **2001**, 115, 6220-6235	3.9	14
37	Solvation effects for polymers at an interface: a hybrid self-consistent field-density functional theory approach. *Journal of Chemical Physics*, **2011**, 135, 204901	3.9	12
36	Nonequilibrium properties of linear polar Kihara fluids from molecular dynamics. Results for models and for liquid acetonitrile. *Journal of Chemical Physics*, **1997**, 107, 2034-2045	3.9	12
35	Dynamical properties and transport coefficients of Kihara linear fluids. *Journal of Chemical Physics*, **1997**, 106, 4753-4767	3.9	12
34	Effect of molecular flexibility of Lennard-Jones chains on vapor-liquid interfacial properties. *Journal of Chemical Physics*, **2014**, 140, 114705	3.9	11
33	Molecular modeling of flexible molecules. Vapor–liquid and fluid–solid equilibria. *Journal of Molecular Liquids*, **2004**, 113, 37-51	6	11
32	Vapour-liquid interfacial properties of square-well chains from density functional theory and Monte Carlo simulation. *Physical Chemistry Chemical Physics*, **2017**, 19, 12296-12309	3.6	10
31	Coarse-graining dipolar interactions in simple fluids and polymer solutions: Monte Carlo studies of the phase behavior. *Physical Chemistry Chemical Physics*, **2009**, 11, 1923-33	3.6	10
30	A computer simulation study of racemic mixtures. *Molecular Physics*, **2002**, 100, 2397-2415	1.7	10

29	Surface van der Waals forces in a nutshell. *Journal of Chemical Physics*, **2019**, 150, 081101	3.9	10
28	Capillary wave theory of adsorbed liquid films and the structure of the liquid-vapor interface. *Physical Review E*, **2017**, 96, 022801	2.4	9
27	Structural transitions and bilayer formation of CTAB aggregates. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2019**, 580, 123730	5.1	9
26	Interfacial free energy of the NaCl crystal-melt interface from capillary wave fluctuations. *Journal of Chemical Physics*, **2015**, 142, 134706	3.9	8
25	Rounded Layering Transitions on the Surface of Ice. *Physical Review Letters*, **2020**, 124, 065702	7.4	8
24	Nanocapillarity and Liquid Bridge-Mediated Force between Colloidal Nanoparticles. *ACS Omega*, **2018**, 3, 112-123	3.9	8
23	Bonded hard-sphere theory and computer simulation of the equation of state of linear fused hard-sphere fluids. *Journal of Chemical Physics*, **2003**, 119, 9633-9639	3.9	8
22	Critical properties of mixtures of alkanes from perturbation theory. *Journal of Chemical Physics*, **1999**, 111, 3183-3191	3.9	8
21	How ice grows from premelting films and water droplets. *Nature Communications*, **2021**, 12, 239	17.4	8
20	Excess properties of mixtures of n-alkanes from perturbation theory. *Journal of Chemical Physics*, **1999**, 111, 3192-3202	3.9	7
19	Premelting of ice adsorbed on a rock surface. *Physical Chemistry Chemical Physics*, **2020**, 22, 11362-11373	3.6	7
18	Structure and water attachment rates of ice in the atmosphere: role of nitrogen. *Physical Chemistry Chemical Physics*, **2019**, 21, 19594-19611	3.6	6
17	Structure and fluctuations of the premelted liquid film of ice at the triple point. *Molecular Physics*, **2019**, 117, 2846-2864	1.7	6
16	Analytic perturbative FMSA equation of state and thermodynamic properties from Monte Carlo simulation of the Kihara potential with a spherical core. *Molecular Physics*, **2015**, 113, 1076-1090	1.7	6
15	Vapour-liquid equilibria of propane and n-alkane conformers. *Molecular Physics*, **1995**, 85, 679-699	1.7	6
14	Towards the Quantitative Prediction of the Phase Behavior of Polymer Solutions by Computer Simulation. *Macromolecular Symposia*, **2009**, 278, 1-9	0.8	5
13	Mesoscopic Hamiltonian for the fluctuations of adsorbed Lennard-Jones liquid films. *Physical Review E*, **2015**, 91, 062404	2.4	4
12	Damped reaction field method and the accelerated convergence of the real space Ewald summation. *Journal of Chemical Physics*, **2014**, 141, 164108	3.9	4

List of Publications

11	Discussion notes on Disjoining pressure of planar adsorbed films by J.R. Henderson. *European Physical Journal: Special Topics*, **2011**, 197, 149-150	2.3	3
10	The vapour - liquid equilibrium ofn-alkanes. *Journal of Physics Condensed Matter*, **1996**, 8, 9643-9648	1.8	3
9	RESEARCH NOTE On the calculation of the frequency sum rules of the heat flux correlation function. *Molecular Physics*, **1999**, 96, 881-884	1.7	2
8	Lifshitz theory of wetting films at three phase coexistence: The case of ice nucleation on Silver Iodide (AgI). *Journal of Colloid and Interface Science*, **2021**, 590, 527-538	9.3	2
7	The vicinity of an equilibrium three-phase contact line using density-functional theory: density profiles normal to the fluid interface. *Molecular Physics*, **2018**, 116, 2239-2243	1.7	2
6	On the calculation of the frequency sum rules of the heat flux correlation function. *Molecular Physics*, **1999**, 96, 881-884	1.7	1
5	Understanding the critical properties of chain molecules		1
4	Crystal growth of bcc titanium from the melt and interfacial properties: A molecular dynamics simulation study. *Journal of Chemical Physics*, **2021**, 154, 184704	3.9	0
3	Discussion notes: Remark on contributions by Binder, Marmur and Sefiane. *European Physical Journal: Special Topics*, **2011**, 197, 245-247	2.3	
2	How Do Droplets Depend on the System Size? Droplet Condensation and Nucleation in Small Simulation Cells **2003**, 125-135		
1	The Droplet Evaporation/Condensation Transition in a Finite Volume. *Springer Proceedings in Physics*, **2004**, 129-133	0.2	