Richard J Sadus

List of Publications by Year in Descending Order

140 papers	2,595 citations	26 h-index	42 g-index
151 ext. papers	2,806 ext. citations	3.2 avg, IF	5.58 L-index

#	Paper	IF	Citations
140	Interatomic Interactions Responsible for the Solid-Liquid and Vapor-Liquid Phase Equilibria of Neon. *Journal of Physical Chemistry B*, **2021**, 125, 8522-8531	3.4	1
139	Ab Initio Interatomic Potentials and the Classical Molecular Simulation Prediction of the Thermophysical Properties of Helium. *Journal of Physical Chemistry B*, **2020**, 124, 2268-2276	3.4	6
138	Vapor-liquid equilibria and cohesive r interactions. *Journal of Chemical Physics*, **2020**, 153, 204504	3.9	1
137	Effect of the range of particle cohesion on the phase behavior and thermodynamic properties of fluids. *Journal of Chemical Physics*, **2020**, 153, 244502	3.9	1
136	Combining intermolecular potentials for the prediction of fluid properties: Two-body and three-body interactions. *Journal of Chemical Physics*, **2020**, 153, 214509	3.9	3
135	The Widom Line and the Lennard-Jones Potential. *Journal of Physical Chemistry B*, **2019**, 123, 8268-8273	3.4	10
134	Molecular simulation of orthobaric isochoric heat capacities near the critical point. *Physical Review E*, **2019**, 99, 012139	2.4	3
133	Flow of water through carbon nanotubes predicted by different atomistic water models. *Journal of Chemical Physics*, **2019**, 150, 194501	3.9	10
132	Two-body interatomic potentials for He, Ne, Ar, Kr, and Xe from ab initio data. *Journal of Chemical Physics*, **2019**, 150, 134504	3.9	16
131	Two-body intermolecular potentials from second virial coefficient properties. *Journal of Chemical Physics*, **2019**, 150, 024503	3.9	7
130	Thermodynamic properties and anomalous behavior of double-Gaussian core model potential fluids. *Physical Review E*, **2019**, 100, 012112	2.4	3
129	Fully a priori prediction of the vapor-liquid equilibria of Ar, Kr, and Xe from ab initio two-body plus three-body interatomic potentials. *Journal of Chemical Physics*, **2019**, 151, 034509	3.9	7
128	Structural behavior of fluids from the vapor and liquid region to the supercritical phase. *Physical Review E*, **2019**, 100, 052132	2.4	5
127	Thermodynamics of Fluid Polyamorphism. *Physical Review X*, **2018**, 8,	9.1	43
126	Intermolecular Potential-Based Equations of State from Molecular Simulation and Second Virial Coefficient Properties. *Journal of Physical Chemistry B*, **2018**, 122, 7757-7763	3.4	8
125	Second virial coefficient properties of the - Lennard-Jones/Mie potential. *Journal of Chemical Physics*, **2018**, 149, 074504	3.9	22
124	Ab initio interatomic potentials and the thermodynamic properties of fluids. *Journal of Chemical Physics*, **2017**, 147, 024505	3.9	11

123	Predicting vapor-liquid phase equilibria with augmented ab initio interatomic potentials. *Journal of Chemical Physics*, **2017**, 146, 244504	3.9	11
122	Atomistic water models: Aqueous thermodynamic properties from ambient to supercritical conditions. *Fluid Phase Equilibria*, **2016**, 407, 7-30	2.5	48
121	Molecular simulation of the thermodynamic, structural, and vapor-liquid equilibrium properties of neon. *Journal of Chemical Physics*, **2016**, 145, 104501	3.9	20
120	Thermophysical properties of supercritical water and bond flexibility. *Physical Review E*, **2015**, 92, 012124	2.4	15
119	Molecular simulation of fluids with non-identical intermolecular potentials: thermodynamic properties of 10-5 + 12-6 Mie potential binary mixtures. *Journal of Chemical Physics*, **2015**, 142, 084504	3.9	12
118	Thermodynamic properties and diffusion of water + methane binary mixtures. *Journal of Chemical Physics*, **2014**, 140, 104505	3.9	16
117	Mg^{2+} coordinating dynamics in Mg:ATP fueled motor proteins. *Journal of Chemical Physics*, **2014**, 140, 115102	3.9	6
116	Thermodynamic properties of supercritical n-m Lennard-Jones fluids and isochoric and isobaric heat capacity maxima and minima. *Journal of Chemical Physics*, **2013**, 139, 154503	3.9	21
115	A suite of domain-specific visual languages for scientific software application modelling **2013**,		8
114	Thermodynamic properties of liquid water from a polarizable intermolecular potential. *Journal of Chemical Physics*, **2013**, 138, 044503	3.9	15
113	Intermolecular interactions and the thermodynamic properties of supercritical fluids. *Journal of Chemical Physics*, **2013**, 138, 194502	3.9	23
112	Intermolecular potentials and the accurate prediction of the thermodynamic properties of water. *Journal of Chemical Physics*, **2013**, 139, 194505	3.9	12
111	Molecular simulation of the phase behavior of fluids and fluid mixtures using the synthetic method. *Journal of Chemical Physics*, **2012**, 137, 054507	3.9	3
110	Dielectric and structural properties of aqueous nonpolar solute mixtures. *Journal of Chemical Physics*, **2012**, 137, 124501	3.9	7
109	Conformational dynamics of ATP/Mg:ATP in motor proteins via data mining and molecular simulation. *Journal of Chemical Physics*, **2012**, 137, 075101	3.9	5
108	Molecular dynamics simulation of the effect of bond flexibility on the transport properties of water. *Journal of Chemical Physics*, **2012**, 137, 104512	3.9	47
107	Structure and polarization properties of water: molecular dynamics with a nonadditive intermolecular potential. *Physical Review E*, **2012**, 85, 051509	2.4	12
106	Nonequilibrium equation of state for Lennard-Jones fluids and the calculation of strain-rate dependent shear viscosity. *AICHE Journal*, **2011**, 57, 250-258	3.6	4

105	Thermodynamic properties in the molecular dynamics ensemble applied to the gaussian core model fluid. *Journal of Chemical Physics*, **2011**, 134, 114515	3.9	21
104	Molecular dynamics simulation of the dielectric constant of water: the effect of bond flexibility. *Journal of Chemical Physics*, **2011**, 134, 234501	3.9	70
103	Allosteric Conformational Transition in Adenylate Kinase: Dynamic Correlations and Implication for Allostery. *Australian Journal of Chemistry*, **2010**, 63, 405	1.2	12
102	Pressure and energy behavior of the Gaussian core model fluid under shear. *Physical Review E*, **2010** , 82, 011201	2.4	7
101	Effect of potential truncations and shifts on the solid-liquid phase coexistence of Lennard-Jones fluids. *Journal of Chemical Physics*, **2010**, 133, 124515	3.9	26
100	Strain-rate dependent shear viscosity of the Gaussian core model fluid. *Journal of Chemical Physics*, **2009**, 131, 224511	3.9	10
99	Solid-liquid phase equilibria of the Gaussian core model fluid. *Journal of Chemical Physics*, **2009**, 131, 184507	3.9	14
98	Phase diagram of the Weeks-Chandler-Andersen potential from very low to high temperatures and pressures. *Physical Review E*, **2009**, 80, 061101	2.4	40
97	Solid-liquid equilibria and triple points of n-6 Lennard-Jones fluids. *Journal of Chemical Physics*, **2009**, 131, 174504	3.9	69
96	A mechanochemical theory for the ATP-fuelled biomolecular motors. *International Journal of Nanotechnology*, **2009**, 6, 1121	1.5	
95	Molecular simulation and theory for nanosystems: Insights for molecular motors. *Molecular Simulation*, **2008**, 34, 23-27	2	3
94	Coarse-grained dynamics of the receiver domain of NtrC: fluctuations, correlations and implications for allosteric cooperativity. *Proteins: Structure, Function and Bioinformatics*, **2008**, 73, 218-27	4.2	11
93	Parallel algorithms for molecular dynamics with induction forces. *Computer Physics Communications* , **2008**, 178, 384-392	4.2	5
92	Role of nonadditive forces on the structure and properties of liquid water. *Journal of Chemical Physics*, **2007**, 127, 154509	3.9	31
91	Influence of bond flexibility on the vapor-liquid phase equilibria of water. *Journal of Chemical Physics*, **2007**, 126, 044701	3.9	40
90	Modified force decomposition algorithms for calculating three-body interactions via molecular dynamics. *Computer Physics Communications*, **2006**, 175, 683-691	4.2	6
89	Analysis of the shape of dendrimers under shear. *Journal of Chemical Physics*, **2006**, 124, 044910	3.9	24
88	Effect of three-body interactions on the vapor-liquid phase equilibria of binary fluid mixtures. *Journal of Chemical Physics*, **2006**, 125, 074503	3.9	19

87	Three-body interactions and solid-liquid phase equilibria: application of a molecular dynamics algorithm. *Physical Review E*, **2006**, 74, 031203	2.4	14
86	Influence of two-body and three-body interatomic forces on gas, liquid, and solid phases. *Physical Review E*, **2006**, 74, 021202	2.4	5
85	Molecular simulation of the thermophysical properties of fluids: phase behaviour and transport properties. *Molecular Simulation*, **2006**, 32, 185-189	2	4
84	Parallelization Algorithms for Three-Body Interactions in Molecular Dynamics Simulation. *Lecture Notes in Computer Science*, **2006**, 374-382	0.9	1
83	Relationships between three-body and two-body interactions in fluids and solids. *Journal of Chemical Physics*, **2006**, 125, 144509	3.9	35
82	Dynamic and coordinating domain motions in the active subunits of the F1-ATPase molecular motor. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2006**, 1764, 1553-60	4	10
81	Molecular simulation of dendrimers and their mixtures under shear: comparison of isothermal-isobaric (NpT) and isothermal-isochoric (NVT) ensemble systems. *Journal of Chemical Physics*, **2005**, 123, 34905	3.9	33
80	A molecular dynamics study of nitric oxide in water: diffusion and structure. *Journal of Chemical Physics*, **2005**, 123, 054505	3.9	35
79	Cooperativity in the motor activities of the ATP-fueled molecular motors. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2005**, 1752, 111-23	4	8
78	Hard sphere compressibility factors for equation of state development. *AICHE Journal*, **2005**, 51, 309-313	3.6	45
77	Molecular simulation of the shear viscosity and the self-diffusion coefficient of mercury along the vapor-liquid coexistence curve. *Journal of Chemical Physics*, **2005**, 123, 34511	3.9	9
76	Response to □Comment on: □New phase for one-component hard spheres□□[J. Chem. Phys. 120, 11686 (2004)]. *Journal of Chemical Physics*, **2004**, 121, 12117-12118	3.9	
75	Viscoelastic properties of dendrimers in the melt from nonequlibrium molecular dynamics. *Journal of Chemical Physics*, **2004**, 121, 12050-9	3.9	51
74	Internal structure of dendrimers in the melt under shear: a molecular dynamics study. *Journal of Chemical Physics*, **2004**, 121, 1091-6	3.9	41
73	Response to □Comment on □Equations of state for fluids: The Dieterici approach revisited□□[J. Chem. Phys. 115, 1460 (2001)]. *Journal of Chemical Physics*, **2004**, 120, 8870-8870	3.9	5
72	Complex cooperativity of ATP hydrolysis in the F(1)-ATPase molecular motor. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2004**, 1698, 197-202	4	8
71	New phase for one-component hard spheres. *Journal of Chemical Physics*, **2004**, 120, 11686-91	3.9	5
70	Global phase diagram for anisotropic binary fluid mixtures: reverse type IV behaviour. *Molecular Physics*, **2003**, 101, 2211-2217	1.7	2

69	New Dieterici-type equations of state for fluid phase equilibria. *Fluid Phase Equilibria*, **2003**, 212, 31-39	2.5	12
68	Phase behaviour of binary fluid mixtures: a global phase diagram solely in terms of pure component properties. *Fluid Phase Equilibria*, **2003**, 214, 67-78	2.5	17
67	Molecular simulation of the vapor–liquid coexistence of mercury. *Journal of Chemical Physics*, **2003**, 119, 6691-6697	3.9	41
66	Scaling behavior for the pressure and energy of shearing fluids. *Physical Review E*, **2003**, 67, 061201	2.4	20
65	Equilibrium and nonequilibrium molecular dynamics methods for determining solid–liquid phase coexistence at equilibrium. *Journal of Chemical Physics*, **2003**, 119, 11017-11023	3.9	21
64	Kinetics and chemomechanical properties of the F1-ATPase molecular motor. *Journal of Chemical Physics*, **2003**, 118, 9890-9898	3.9	24
63	Molecular simulation of liquid-crystal transitions in hard prolate ellipsoid monomers and dimers. *Fluid Phase Equilibria*, **2002**, 194-197, 227-231	2.5	2
62	The Dieterici alternative to the van der Waals approach for equations of state: second virial coefficients. *Physical Chemistry Chemical Physics*, **2002**, 4, 919-921	3.6	23
61	Beyond Traditional Effective Intermolecular Potentials and Pairwise Interactions in Molecular Simulation. *Lecture Notes in Computer Science*, **2002**, 932-941	0.9	3
60	The strain rate dependence of shear viscosity, pressure and energy from two-body and three-body interactions. *Fluid Phase Equilibria*, **2001**, 183-184, 371-379	2.5	10
59	Energy and pressure of shearing fluids at different state points. *Physical Review E*, **2001**, 64, 021201	2.4	14
58	Liquid-crystal behavior of hard ellipsoid dimers. *Journal of Chemical Physics*, **2001**, 114, 5432-5434	3.9	6
57	Equations of state for fluids: The Dieterici approach revisited. *Journal of Chemical Physics*, **2001**, 115, 1460-1462	3.9	34
56	Analytic dependence of the pressure and energy of an atomic fluid under shear. *Physical Review E*, **2001**, 63, 021204	2.4	31
55	On the relationship between two-body and three-body interactions from nonequilibrium molecular dynamics simulation. *Journal of Chemical Physics*, **2001**, 115, 9410-9413	3.9	22
54	Molecular simulation of the vapour–liquid phase coexistence of neon and argon using ab initio potentials. *Physical Chemistry Chemical Physics*, **2001**, 3, 1297-1302	3.6	38
53	Three-body interactions and the phase equilibria of mixtures. *High Temperatures - High Pressures*, **2001**, 33, 111-118	1.3	5
52	Equations of state for the calculation of fluid-phase equilibria. *AICHE Journal*, **2000**, 46, 169-196	3.6	298

51	Molecular simulation of the high-pressure phase equilibria of binary atomic fluid mixtures using the exponential-6 intermolecular potential. *Fluid Phase Equilibria*, **2000**, 170, 269-284	2.5	11
50	Closed-loop liquid-liquid equilibria and the global phase behaviour of binary mixtures involving hard-sphere + van der Waals interactions. *Molecular Physics*, **2000**, 98, 715-723	1.7	22
49	A link between the two-body and three-body interaction energies of fluids from molecular simulation. *Journal of Chemical Physics*, **2000**, 112, 6382-6385	3.9	38
48	Phase behaviour of carbon dioxide–benzene–water ternary mixtures at high pressures and temperatures up to 300 MPa and 600 K. *Physical Chemistry Chemical Physics*, **2000**, 2, 4157-4164	3.6	6
47	Molecular simulation of the phase behaviour of ternary fluid mixtures: the effect of a third component on vapour–liquid and liquid–liquid coexistence. *Fluid Phase Equilibria*, **1999**, 157, 169-180	2.5	10
46	Simple equation of state for hard-sphere chains. *AICHE Journal*, **1999**, 45, 2454-2457	3.6	12
45	An equation of state for hard convex body chains. *Molecular Physics*, **1999**, 97, 1279-1284	1.7	2
44	Phase behaviour of ternary mixtures: a theoretical investigation of the critical properties of mixtures with equal size components. *Physical Chemistry Chemical Physics*, **1999**, 1, 4329-4336	3.6	6
43	Molecular simulation of the phase behavior of noble gases using accurate two-body and three-body intermolecular potentials. *Journal of Chemical Physics*, **1999**, 111, 1533-1540	3.9	90
42	Exact calculation of the effect of three-body Axilrod–Teller interactions on vapour–liquid phase coexistence. *Fluid Phase Equilibria*, **1998**, 144, 351-359	2.5	33
41	The effect of three-body interactions on the liquid–liquid phase coexistence of binary fluid mixtures. *Fluid Phase Equilibria*, **1998**, 150-151, 63-72	2.5	11
40	Effect of Three-Body Interactions between Dissimilar Molecules on the Phase Behavior of Binary Mixtures: The Transition from Vapor–Liquid Equilibria to Type III Behavior. *Industrial & Engineering Chemistry Research*, **1998**, 37, 2977-2982	3.9	7
39	Molecular Simulation of Henry's Constant at Vapor–Liquid and Liquid–Liquid Phase Boundaries. *Journal of Physical Chemistry B*, **1997**, 101, 3834-3838	3.4	16
38	Molecular simulation of intermolecular attraction and repulsion in coexisting liquid and vapour phases. *Fluid Phase Equilibria*, **1997**, 134, 77-85	2.5	13
37	Molecular simulation of the vapour-liquid equilibria of pure fluids and binary mixtures containing dipolar components: the effect of Keesom interactions. *Molecular Physics*, **1996**, 87, 979-990	1.7	27
36	RESEARCH NOTE Molecular simulation of the liquid-liquid equilibria of binary mixtures containing dipolar and non-polar components interacting via the Keesom potential. *Molecular Physics*, **1996**, 89, 1187-1194	1.7	12
35	Monte Carlo simulation of vapour-liquid equilibria in Lennard-Jones + three-body potential binary fluid mixtures. *Fluid Phase Equilibria*, **1996**, 116, 289-295	2.5	4
34	Vapour-liquid and liquid-liquid phase equilibria of binary mixtures containing helium: comparison of experiment with predictions using equations of state. *Fluid Phase Equilibria*, **1996**, 122, 1-15	2.5	19

33	Binary mixtures of water + five noble gases: comparison of binodal and critical curves at high pressures. *Fluid Phase Equilibria*, **1996**, 123, 1-15	2.5	1
32	A Simplified Thermodynamic Perturbation Theory-Dimer Equation of State for Mixtures of Hard-Sphere Chains. *Macromolecules*, **1996**, 29, 7212-7216	5.5	7
31	Three-body interactions in fluids from molecular simulation: Vapor–liquid phase coexistence of argon. *Journal of Chemical Physics*, **1996**, 104, 4784-4787	3.9	34
30	Prediction of one-component vapour-liquid equilibria from the triple point to the critical point using a simplified perturbed hard-chain theory equation of state. *Fluid Phase Equilibria*, **1995**, 109, 171-182	2.5	4
29	High-Pressure Phase Equilibria and Critical Curve of the Water + Helium System to 200 MPa and 723 K. *The Journal of Physical Chemistry*, **1995**, 99, 4273-4277		25
28	Equations of State for Hard-Sphere Chains. *The Journal of Physical Chemistry*, **1995**, 99, 12363-12366		25
27	Calculating one-component vapour-liquid equilibria using equations of state: a new temperature-dependence for the attractive term in the Christoforakos-Franck equation. *Fluid Phase Equilibria*, **1995**, 103, 41-50	2.5	2
26	Influence of molecular shape on vapour-liquid equilibria. *Fluid Phase Equilibria*, **1994**, 95, 371-381	2.5	3
25	Calculating critical transitions of fluid mixtures: Theory vs. experiment. *AICHE Journal*, **1994**, 40, 1376-1403	3.6	72
24	Calculation of the critical high pressure liquid-liquid phase equilibria of binary mixtures containing ammonia Unlike interaction parameters for the Heilig–Franck equation of state. *Fluid Phase Equilibria*, **1994**, 101, 89-99	2.5	4
23	Influence of combining rules and molecular shape on the high pressure phase equilibria of binary fluid mixtures. *The Journal of Physical Chemistry*, **1993**, 97, 1985-1992		14
22	High-pressure phase equilibria and supercritical pVT data of the binary water + methane mixture to 723 K and 200 MPa. *The Journal of Physical Chemistry*, **1993**, 97, 9054-9059		73
21	Novel high pressure critical phase transitions in multicomponent fluid mixtures. *Fluid Phase Equilibria*, **1993**, 83, 101-108	2.5	7
20	Influence of quantum effects on the high-pressure phase behavior of binary mixtures containing hydrogen. *The Journal of Physical Chemistry*, **1992**, 96, 3855-3860		12
19	Novel critical transitions in ternary fluid mixtures. *The Journal of Physical Chemistry*, **1992**, 96, 5197-5202		9
18	Predicting the Gas-Liquid Critical Properties of Binary Mixtures: An Alternative to Conventional Mixing Rules. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1992**, 96, 1454-1459		11
17	MODELS FOR HIGH PRESSURE MULTICOMPONENT EQUILIBRIA **1992**, 25-68		2
16	SURVEY OF THE HIGH PRESSURE PHASE BEHAVIOUR OF FLUIDS **1992**, 1-12		11

15	PROCEDURE FOR DETERMINING THE PHASE BEHAVIOUR OF TERNARY MIXTURES: COMPARISON OF EXPERIMENT WITH THEORY FOR GAS-LIQUID CRITICAL TEMPERATURES **1992**, 69-85		
14	NOVEL HIGHER ORDER CRITICAL PHENOMENA IN TERNARY MIXTURES **1992**, 87-102		
13	Unusual critical temperature phenomena in fluid mixtures containing perfluorotributylamine. *Fluid Phase Equilibria*, **1992**, 77, 269-283	2.5	2
12	TERNARY TETRAFLUOROMETHANE AND n-ALKANE MIXTURES **1992**, 177-204		
11	TERNARY MIXTURES CONTAINING WATER AND n-ALKANES **1992**, 229-255		
10	Phase behaviour of 1-alkanol + alkane mixtures: gas-liquid critical temperatures. *Fluid Phase Equilibria*, **1991**, 67, 259-271	2.5	7
9	Attractive forces in binary mixtures: a priori prediction of gas-liquid critical properties. *The Journal of Physical Chemistry*, **1989**, 93, 3787-3790		11
8	Gas-liquid critical properties of binary mixtures of n-alkanes and 2,2,4-trimethylpentane with the weakly polar halocarbons 1,2-dichloroethane, cis-1,2-dichloroethene trans-1,2-dichloroethene and tetrachloromethane. *Industrial & Engineering Chemistry Research*, **1989**, 28, 481-484	3.9	7
7	Critical properties of ternary mixtures: Siloxane and perfluoromethylcyclohexane mixtures. *Chemical Engineering Science*, **1988**, 43, 883-885	4.4	11
6	Deiters' equation of state and critical phenomena. *Chemical Engineering Science*, **1988**, 43, 459-466	4.4	14
5	Application of hard convex body and hard sphere equations of state to the critical properties of binary mixtures. *Fluid Phase Equilibria*, **1988**, 39, 89-99	2.5	19
4	Prediction of binary and ternary critical properties using deiters' equation, hard sphere and hard convex body equations of state. *Fluid Phase Equilibria*, **1988**, 42, 85-103	2.5	4
3	Critical properties of ternary mixtures: hydrocarbon, acetone and alkanenitrile mixtures. *Chemical Engineering Science*, **1987**, 42, 1717-1722	4.4	18
2	Phase behaviour of fluorocarbon and hydrocarbon mixtures: interpretation of type II and type III behaviour in terms of a hard-sphere + attractive force equation of state. *Fluid Phase Equilibria*, **1986**, 25, 263-272	2.5	18
1	Molecular simulation of the vapour-liquid equilibria of pure fluids and binary mixtures containing dipolar components: the effect of Keesom interactions		5