

CITATION REPORT

List of articles citing

Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble

DOI: 10.1080/00268978700101491
Molecular Physics, 1987, 61, 813-826.

Source: <https://exaly.com/paper-pdf/19129748/citation-report.pdf>

Version: 2024-04-10

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
1779	Cooperative Catalysis by Surface Lewis Acid/Silanol for Selective Fructose Etherification on Sn-SPP Zeolite.		
1778	Reproducing Quantum Probability Distributions at the Speed of Classical Dynamics: A New Approach for Developing Force-Field Functors.		
1777	Computational Design of High Block Oligomers for Accessing 1 nm Domains.		
1776	Brick-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method.		
1775	Petroleum on the continental shelves. 1947 , 42, 83-85		
1774	Vapour-liquid critical lines predicted by distribution function theories. <i>Molecular Physics</i> , 1987 , 62, 3-18	1.7	9
1773	Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble. <i>Molecular Physics</i> , 1987 , 62, 701-719	1.7	268
1772	Off-lattice Monte Carlo simulations of polymer melts confined between two plates. <i>Journal of Chemical Physics</i> , 1988 , 89, 5206-5215	3.9	217
1771	Phase equilibria by simulation in the Gibbs ensemble. <i>Molecular Physics</i> , 1988 , 63, 527-545	1.7	976
1770	The density profile of a confined fluid. <i>Molecular Physics</i> , 1988 , 63, 159-163	1.7	53
1769	Monte Carlo simulation of multicomponent equilibria in a semigrand canonical ensemble. <i>Molecular Physics</i> , 1988 , 64, 1105-1131	1.7	211
1768	Critical behavior of the hypernetted-chain equation for a Lennard-Jones mixture. 1989 , 40, 6384-6387		15
1767	Relationships in the approach to criticality in fluids, including systematic differences between vapor-liquid and liquid-liquid systems. <i>Journal of Chemical Physics</i> , 1989 , 90, 5742-5748	3.9	33
1766	Phase stability of multicomponent highly asymmetric electrolytes: A charged hard sphere model study. <i>Journal of Chemical Physics</i> , 1989 , 91, 4902-4908	3.9	14
1765	Phase stability of dense charged hard sphere fluid mixtures. <i>Journal of Chemical Physics</i> , 1989 , 90, 1091-1098	3.9	28
1764	Phase Equilibria of Quadrupolar Fluids by Simulation in the Gibbs Ensemble. 1989 , 2, 147-162		47
1763	Phase diagrams of interaction site fluids. <i>Molecular Physics</i> , 1989 , 67, 33-52	1.7	50

1762	Application of the Gibbs ensemble to the study of fluid-fluid phase equilibrium in a binary mixture of symmetric non-additive hard spheres. <i>Molecular Physics</i> , 1989 , 67, 739-745	1.7	69
1761	Gibbs ensemble simulation of phase equilibrium in the hard core two-Yukawa fluid model for the Lennard-Jones fluid. <i>Molecular Physics</i> , 1989 , 68, 629-635	1.7	38
1760	Molecular dynamics studies for the new refrigerant R152a with simple model potentials. <i>Molecular Physics</i> , 1989 , 68, 1079-1093	1.7	46
1759	Phase equilibria for fluid mixtures from monte-carlo simulation. <i>Fluid Phase Equilibria</i> , 1989 , 53, 177-189	2.5	100
1758	Food colloid science and the art of computer simulation. 1989 , 3, 345-363		4
1757	Molecular dynamics simulation using hard particles. 1989 , 9, 301-353		100
1756	The gibbs method for molecular-based computer simulations of phase equilibria. <i>Fluid Phase Equilibria</i> , 1989 , 53, 133-141	2.5	38
1755	Some interesting properties of vapor-liquid or liquid-liquid coexistence curves for ionic and non-ionic fluids. 1989 , 139, 25-32		8
1754	Fluids, both ionic and non-ionic, over wide ranges of temperature and composition. 1989 , 21, 1-17		9
1753	Exact calculations of fluid-phase equilibria by Monte Carlo simulation in a new statistical ensemble. 1989 , 10, 447-457		96
1752	Computer simulations in the Gibbs ensemble. <i>Molecular Physics</i> , 1989 , 68, 931-950	1.7	286
1751	Calculation of the chemical potential in the Gibbs ensemble. <i>Molecular Physics</i> , 1989 , 68, 951-958	1.7	161
1750	Vapour-liquid equilibria for Stockmayer fluids. <i>Molecular Physics</i> , 1989 , 68, 765-769	1.7	85
1749	The Role of Computer Simulation in Studying Fluid Phase Equilibria. 1989 , 2, 223-252		73
1748	A theory of fluids reliable in the critical region. 1990 , 12, 419-426		3
1747	Analysis of infinite dilution partial molar volumes using a distribution function theory. <i>Fluid Phase Equilibria</i> , 1990 , 57, 227-247	2.5	63
1746	Theory of critical phenomena in fluids. <i>Journal of Physics Condensed Matter</i> , 1990 , 2, SA121-SA125	1.8	4
1745	Application of excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble. <i>Journal of Chemical Physics</i> , 1990 , 92, 1285-1293	3.9	62

1744	Orthobaric Densities from Simulations of the Liquid Vapour Interface. 1990 , 5, 233-243		25
1743	The gas-liquid transition of the two-dimensional Lennard-Jones fluid. <i>Journal of Physics Condensed Matter</i> , 1990 , 2, 7009-7032	1.8	122
1742	Differential approach to the theory of fluids. 1990 , 42, 6104-6115		50
1741	Wetting transitions at the argon-solid-CO ₂ interface: Molecular-dynamics studies. 1990 , 41, 6866-6870		50
1740	Correlation of Zeno (Z = 1) Line for Supercritical Fluids with Vapor-Liquid Rectilinear Diameters. 1990 , 30, 59-68		39
1739	Rotational insertion bias: a novel method for simulating dense phases of structured particles, with particular application to water. <i>Molecular Physics</i> , 1990 , 71, 931-943	1.7	96
1738	Fluid-Fluid Phase Separation in a Repulsive Lennard-Jones Mixture: A Comparison with the Full Lennard-Jones Mixture by Means of Computer Simulations. 1990 , 13, 679-683		43
1737	Liquid-vapour coexistence of the Gay-Berne fluid by Gibbs-ensemble simulation. <i>Molecular Physics</i> , 1990 , 71, 1223-1231	1.7	70
1736	Phase equilibria in polydisperse fluids. <i>Journal of Chemical Physics</i> , 1990 , 92, 4456-4467	3.9	42
1735	Vapour-liquid equilibria for quadrupolar Lennard-Jones fluids. <i>Journal of Physics Condensed Matter</i> , 1990 , 2, 4281-4288	1.8	46
1734	Monte Carlo simulation of phase equilibria for the two-dimensional Lennard-Jones fluid in the Gibbs ensemble. <i>Journal of Chemical Physics</i> , 1990 , 92, 5463-5466	3.9	50
1733	Stochastic Methods. 1990 , 51-103		2
1732	Vapour liquid equilibrium of a pure fluid from test particle method in combination with NpT molecular dynamics simulations. <i>Molecular Physics</i> , 1990 , 69, 463-473	1.7	123
1731	Molecular Simulations of Methane Adsorption in Silicalite. 1991 , 8, 73-92		53
1730	An Introduction to Molecular Dynamics, with Applications to the Glass Transition. 1991 , 3-20		1
1729	Vapor-liquid equilibria of the two-dimensional Lennard-Jones fluid(s). <i>Journal of Chemical Physics</i> , 1991 , 94, 5663-5668	3.9	130
1728	Monte Carlo: Choosing Which Game to Play. 1991 , 67-84		2
1727	Lecture Notes on: Free-Energy Calculations. 1991 , 85-117		10

1726	Liquid crystal phase diagram of the Gay-Berne fluid. <i>Molecular Physics</i> , 1991 , 74, 405-424	1.7	235
1725	9 Future Opportunities in Thermodynamics. 1991 , 16, 169-189		
1724	Solid-Fluid Coexistence in Binary Hard Sphere Mixtures by Semigrand Monte Carlo Simulation. 1991 , 7, 285-302		49
1723	7 Thermodynamics. 1991 , 16, 125-154		1
1722	Monte Carlo Simulations of Growth Kinetics and Phase Transitions at Interfaces: Some Recent Results. 1991 , 237, 37		
1721	Liquid-liquid and liquid-vapor separation in hard sphere Yukawa mixtures. 1991 , 158, 325-330		13
1720	Evaluation of a statistical-mechanical virial equation of state, using Gibbs-ensemble molecular simulations. <i>Fluid Phase Equilibria</i> , 1991 , 66, 41-55	2.5	9
1719	Investigation of the transition to liquid-liquid immiscibility for Lennard-Jones (12,6) systems, using Gibbs-ensemble molecular simulations. <i>Fluid Phase Equilibria</i> , 1991 , 66, 57-75	2.5	33
1718	Phase equilibria and chemical potentials in infinite dilution of non-ideal fluid mixtures from perturbation theory. <i>Fluid Phase Equilibria</i> , 1991 , 67, 151-171	2.5	5
1717	Monte Carlo studies of binary mixtures: A fast algorithm for equilibration. 1991 , 187, 8-12		4
1716	How good is conformal solutions theory for phase equilibrium predictions?. <i>Fluid Phase Equilibria</i> , 1991 , 65, 1-18	2.5	82
1715	Equations of state from generalized perturbation theory. <i>Fluid Phase Equilibria</i> , 1991 , 67, 127-150	2.5	11
1714	Effect of molecular elongation on liquid-vapour properties: computer simulation and virial approximation. 1991 , 177, 174-181		21
1713	Vapour-liquid equilibria of the hard core Yukawa fluid. <i>Molecular Physics</i> , 1991 , 74, 35-39	1.7	38
1712	A Molecular Simulation of A Liquid-crystal Model. 1991 , 7, 357-385		74
1711	Computer simulation of fluid-fluid phase coexistence in mixtures of nonadditive soft disks. <i>Journal of Chemical Physics</i> , 1991 , 94, 2238-2243	3.9	21
1710	Fluid-fluid phase separation of nonadditive hard-sphere mixtures as predicted by integral-equation theories. <i>Journal of Chemical Physics</i> , 1991 , 95, 4565-4579	3.9	68
1709	Monte Carlo simulation of equilibrium chemical composition of molecular fluid mixtures in the Natoms PT ensemble. <i>Journal of Chemical Physics</i> , 1991 , 94, 7550-7553	3.9	37

1708	Critical line of He-H ₂ up to 2500 K and the influence of attraction on fluid-fluid separation. 1991 , 44, 6630-6634		22
1707	Square-well diatomics: Bulk equation of state, density profiles near walls, virial coefficients and coexistence properties. <i>Molecular Physics</i> , 1991 , 72, 619-641	1.7	59
1706	On the equation of state of charged colloidal systems. <i>Journal of Chemical Physics</i> , 1991 , 94, 5083-5089	3.9	32
1705	A Modified Gibbs Ensemble Method for Calculating Fluid Phase Equilibria. 1991 , 7, 97-103		10
1704	Molecular dynamics simulations of wetting and drying in LJ models of solid-fluid interfaces in the presence of liquid-vapour coexistence. <i>Molecular Physics</i> , 1991 , 73, 1383-1399	1.7	42
1703	Hard ellipsoids of revolution with square wells: a comparison between computer simulation and theory in the liquid-vapour region. <i>Molecular Physics</i> , 1992 , 76, 1275-1279	1.7	19
1702	Thermodynamic Data. 1992 ,		2
1701	Chain length and density dependence of the chemical potential of lattice polymers. <i>Journal of Chemical Physics</i> , 1992 , 97, 6666-6673	3.9	21
1700	A method of molecular simulation of free energy. <i>Journal of Chemical Physics</i> , 1992 , 96, 9046-9049	3.9	5
1699	Gibbs Ensemble Calculations with an Equation of State: An Application to Vapor-Liquid Equilibria. 1992 , 9, 223-238		9
1698	Capillary condensation in the lattice gas model: A Monte Carlo study. <i>Journal of Chemical Physics</i> , 1992 , 96, 1444-1454	3.9	103
1697	Thermodynamics, statistical thermodynamics, and computer simulation of crystals with vacancies and interstitials. 1992 , 46, 4539-4548		47
1696	Phase equilibria and critical behavior of square-well fluids of variable width by Gibbs ensemble Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 1992 , 96, 2296-2305	3.9	278
1695	Effect of a density-dependent potential on the phase behaviour of fluids. <i>Molecular Physics</i> , 1992 , 77, 1021-1031	1.7	36
1694	Theoretical Calculation of the Liquid-Vapor Coexistence Curve of Water, Chloroform and Methanol with the Cavity-Biased Monte Carlo Method in the Gibbs Ensemble. 1992 , 9, 257-267		48
1693	Simulation results and corresponding states correlation for pure rigid molecular fluids. <i>Molecular Physics</i> , 1992 , 77, 351-379	1.7	9
1692	Phase equilibria for associating Lennard-Jones fluids from theory and simulation. <i>Molecular Physics</i> , 1992 , 77, 1033-1053	1.7	84
1691	Calculation of Vapour-Liquid Equilibria of Lennard-Jones Binary Systems by the Gibbs Ensemble Monte Carlo Simulation. 1992 , 8, 297-304		4

1690	Interbilayer repulsion in nonionic surfactant-water lamellar phases.. <i>Molecular Physics</i> , 1992 , 75, 1023-1038	3
1689	Computer Simulation Study of Adsorption, Isothermic Heat and Phase Transitions of Methane on Graphite. 1992 , 290, 191	2
1688	MODELS FOR HIGH PRESSURE MULTICOMPONENT EQUILIBRIA. 1992 , 25-68	2
1687	SURVEY OF THE HIGH PRESSURE PHASE BEHAVIOUR OF FLUIDS. 1992 , 1-12	11
1686	Bulk and interfacial properties of polar and molecular fluids. 1992 , 45, 7330-7354	100
1685	Recent progress in the simulation of classical fluids. 1992 , 121-204	4
1684	Monte Carlo-Self Consistent Field Study of the Symmetrical Models of Polyelectrolytes. 1992 , 9, 285-306	14
1683	Direct Determination of Fluid Phase Equilibria by Simulation in the Gibbs Ensemble: A Review. 1992 , 9, 1-23	309
1682	A grand ensemble Monte Carlo study of metal adsorption on a (110) bcc substrate. 1992 , 264, 455-466	6
1681	Vapour liquid equilibria of the Lennard-Jones fluid from the NpT plus test particle method. <i>Molecular Physics</i> , 1992 , 76, 1319-1333	1.7 372
1680	Configurational bias Monte Carlo: a new sampling scheme for flexible chains. <i>Molecular Physics</i> , 1992 , 75, 59-70	1.7 912
1679	Finite size effects for the simulation of phase coexistence in the Gibbs ensemble near the critical point. <i>Journal of Chemical Physics</i> , 1992 , 96, 6989-6995	3.9 98
1678	Computer Simulations of Aqueous Fluids at High Temperatures and Pressures. 1992 , 1-59	5
1677	Direct simulation of phase equilibria of chain molecules. <i>Journal of Physics Condensed Matter</i> , 1992 , 4, L255-L259	1.8 165
1676	Phase equilibrium in liquid binary mixtures of non-additive hard spheres. 1992 , T45, 251-252	7
1675	Molecular Dynamics Simulations of Liquids and Solutions. 1992 , 57-132	
1674	Vapor-liquid equilibria for polyatomic fluids from site-site computer simulations: pure hydrocarbons and binary mixtures containing methane. <i>Fluid Phase Equilibria</i> , 1992 , 73, 187-210	2.5 52
1673	Molecular simulation of phase equilibria: simple, ionic and polymeric fluids. <i>Fluid Phase Equilibria</i> , 1992 , 76, 97-112	2.5 115

1672	A simple equation of state for the Lennard-Jones fluid. <i>Fluid Phase Equilibria</i> , 1992 , 77, 13-38	2.5	17
1671	Can the Van der Waals loop vanish?. 1992 , 199, 403-407		8
1670	Recent vapour pressure equations for the Lennard-Jones fluid based on molecular simulations. <i>Fluid Phase Equilibria</i> , 1993 , 89, 383-385	2.5	8
1669	Molecular simulation of self-assembly in surfactant and protein solutions. <i>Fluid Phase Equilibria</i> , 1993 , 82, 251-260	2.5	13
1668	Gibbs ensemble simulation of mixed solvent electrolyte solutions. <i>Fluid Phase Equilibria</i> , 1993 , 86, 147-172	2.5	12
1667	Molecular simulation of the enthalpies of argon (1) + methane (2) at different temperatures and pressures. 1993 , 221, 163-170		4
1666	Adhesive-hard-sphere approximation for vapor/liquid transitions in colloidal dispersions. 1993 , 81, 181-193		14
1665	Simulating the critical behaviour of complex fluids. 1993 , 365, 330-332		406
1664	Does C60 have a liquid phase?. 1993 , 365, 425-426		251
1663	Simulation studies of gas-liquid transitions in two dimensions via a subsystem-block-density distribution analysis. <i>European Physical Journal B</i> , 1993 , 90, 215-228	1.2	51
1662	An equation of state for lennard-jones pure fluids applicable over a very wide temperature range. <i>Fluid Phase Equilibria</i> , 1993 , 85, 71-80	2.5	18
1661	Applications of molecular simulation. <i>Fluid Phase Equilibria</i> , 1993 , 83, 1-14	2.5	19
1660	Computer simulation of vapor-liquid equilibrium in mixed solvent electrolyte solutions. <i>Fluid Phase Equilibria</i> , 1993 , 83, 213-222	2.5	15
1659	Chemical potentials in ionic systems from Monte Carlo simulations with distance-biased test particle insertions. <i>Fluid Phase Equilibria</i> , 1993 , 83, 223-231	2.5	13
1658	Molecular dynamics and Monte Carlo simulations in the grand canonical ensemble: Local versus global control. <i>Journal of Chemical Physics</i> , 1993 , 98, 4897-4908	3.9	73
1657	Computer Simulations in the Gibbs Ensemble. 1993 , 173-209		8
1656	The Monte Carlo Method. 1993 , 1-22		4
1655	Advanced Monte Carlo Techniques. 1993 , 93-152		11

1654	Eight physical systems of thermodynamics, statistical mechanics, and computer simulations. <i>Molecular Physics</i> , 1993 , 80, 1183-1193	1.7	27
1653	Gibbs-Duhem integration: a new method for direct evaluation of phase coexistence by molecular simulation. <i>Molecular Physics</i> , 1993 , 78, 1331-1336	1.7	290
1652	A new potential for the numerical simulations of electrolyte solutions on a hypersphere. <i>Journal of Chemical Physics</i> , 1993 , 99, 8953-8963	3.9	42
1651	Vapour-liquid equilibria for two centre Lennard-Jones diatomics and dipolar diatomics. <i>Molecular Physics</i> , 1993 , 80, 997-1007	1.7	44
1650	Locating liquid-solid transitions in computer simulations based on local structure analysis. <i>Journal of Physics Condensed Matter</i> , 1993 , 5, 8509-8522	1.8	17
1649	Direct evaluation of phase coexistence by molecular simulation via integration along the saturation line. <i>Journal of Chemical Physics</i> , 1993 , 98, 4149-4162	3.9	515
1648	Monte Carlo simulation of lipid mixtures: finding phase separation. 1993 , 65, 1788-94		53
1647	A critical study of the simulation of the liquid-vapour interface of a Lennard-Jones fluid. <i>Molecular Physics</i> , 1993 , 78, 437-459	1.7	157
1646	The Lennard-Jones equation of state revisited. <i>Molecular Physics</i> , 1993 , 78, 591-618	1.7	1124
1645	Finite-size effects and approach to criticality in Gibbs ensemble simulations. <i>Molecular Physics</i> , 1993 , 80, 843-852	1.7	59
1644	Calculation of Solvation Free-Energy Differences for Large Solute Change from Computer Simulations with Quadrature-Based Nearly Linear Thermodynamic Integration. 1993 , 10, 225-239		21
1643	Implementation of the Gibbs ensemble using a thermodynamic model for one of the coexisting phases. <i>Molecular Physics</i> , 1993 , 79, 39-52	1.7	11
1642	Vapour-liquid equilibria of stockmayer fluids. <i>Molecular Physics</i> , 1993 , 78, 271-283	1.7	75
1641	Phase diagram of simple fluids: a comprehensive theoretical approach. <i>Journal of Physics Condensed Matter</i> , 1993 , 5, B75-B82	1.8	34
1640	Computer simulation of critical phenomena in fluids. <i>Journal of Physics Condensed Matter</i> , 1993 , 5, B193-B200		10
1639	Further studies of prewetting transitions via Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 1993 , 99, 6897-6906	3.9	48
1638	Nucleation in dipolar fluids: Stockmayer fluids. <i>Journal of Chemical Physics</i> , 1993 , 99, 4670-4679	3.9	45
1637	Estimation of free energy via single particle sampling in Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1993 , 98, 1531-1533	3.9	5

1636	What makes a polar liquid a liquid?. 1993 , 71, 3991-3994		253
1635	Search of the gas-liquid transition of dipolar hard spheres. <i>Journal of Chemical Physics</i> , 1993 , 98, 9835-9849		134
1634	Path-integral Monte Carlo study of a model adsorbate with internal quantum states. 1993 , 47, 7788-7804		30
1633	A computer simulation study of the liquid-vapor coexistence curve of water. <i>Journal of Chemical Physics</i> , 1993 , 98, 8221-8235	3.9	324
1632	Phase stability of dense multicomponent charged and uncharged hard-sphere fluid mixtures. <i>Journal of Chemical Physics</i> , 1993 , 98, 1579-1587	3.9	11
1631	Prediction of the phase diagram of rigid C60 molecules. 1993 , 71, 1200-1203		165
1630	Monte Carlo studies of finite-size scaling in the Gibbs ensemble at criticality for the two-dimensional Ising model. 1993 , 47, 5497-5499		8
1629	Monte Carlo simulation of adsorption of gases in carbonaceous slitlike pores.. 1993 , 26, 266-272		22
1628	Microscopic theoretical description of phase stability in hard sphere Yukawa mixtures. <i>Molecular Physics</i> , 1993 , 78, 83-93	1.7	16
1627	The Effect of the Combined Volume on the Efficiency of Gibbs Ensemble Simulations. 1993 , 11, 395-397		2
1626	Chemical equilibrium in high pressure molecular fluid mixtures. 1994 ,		2
1625	Fluid-fluid phase separation in binary mixtures of asymmetric non-additive hard spheres. <i>Journal of Physics Condensed Matter</i> , 1994 , 6, A163-A166	1.8	29
1624	Molecular dynamics simulation of the chemical potentials of mixtures. <i>Molecular Physics</i> , 1994 , 83, 779-787		6
1623	Phase Diagrams of Diatomic Molecules Using the Gibbs Ensemble Monte Carlo Method. 1994 , 13, 11-24		32
1622	A direct method for determination of chemical potential with molecular dynamics simulations. <i>Molecular Physics</i> , 1994 , 82, 841-855	1.7	15
1621	The liquid-vapour coexistence of charged hard spheres. <i>Journal of Physics Condensed Matter</i> , 1994 , 6, A171-A174	1.8	2
1620	Computer simulation of late-stage growth in phase-separating binary mixtures: critical and off-critical quenches. <i>Journal of Physics Condensed Matter</i> , 1994 , 6, A205-A209	1.8	14
1619	Peculiarities in the high-pressure phase behaviour of binary mixtures of nitrogen with methane, helium and water. <i>Journal of Physics Condensed Matter</i> , 1994 , 6, A187-A192	1.8	5

1618	Deviation from corresponding-states behaviour for polar fluids. <i>Molecular Physics</i> , 1994 , 82, 383-392	1.7	40
1617	Phase transitions in simple fluids: An application of a one-phase entropic criterion to Lennard-Jones and point Yukawa fluids. 1994 , 49, 5164-5168		18
1616	Phase equilibria of Lennard-Jones dipolar plus quadrupolar fluids by Gibbs-ensemble Monte Carlo simulation. 1994 , 49, 2175-2183		10
1615	Vapor-liquid and liquid-liquid phase equilibria of mixtures containing square-well molecules by Gibbs ensemble Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 1994 , 101, 3190-3204	3.9	63
1614	Molecular dynamics implementation of the Gibbs ensemble calculation. <i>Journal of Chemical Physics</i> , 1994 , 101, 10899-10907	3.9	30
1613	Computer simulation of vapor-liquid equilibria of linear quadrupolar fluids. Departures from the principle of corresponding states. <i>Journal of Chemical Physics</i> , 1994 , 101, 4166-4176	3.9	39
1612	Stability of fluids with more than two components. <i>Molecular Physics</i> , 1994 , 83, 1171-1190	1.7	21
1611	Exploring the influence of three-body classical dispersion forces on phase equilibria of simple fluids: An integral-equation approach. 1994 , 49, 402-409		11
1610	High-temperature phase diagram of the fullerene C ₆₀ . 1994 , 50, 1301-1304		44
1609	Phase diagram of a model anticlustering binary mixture in two dimensions: A semi-grand-canonical Monte Carlo study. 1994 , 49, 1468-1477		14
1608	Monte Carlo evaluation of ensemble averages involving particle number variations in dense fluid systems. <i>Journal of Chemical Physics</i> , 1994 , 101, 4986-4994	3.9	29
1607	Derivation of Stockmayer potential parameters for polar fluids. <i>Fluid Phase Equilibria</i> , 1994 , 99, 1-18	2.5	181
1606	Thermophysical properties: What have we learned recently, and what do we still need to know?. 1994 , 15, 1013-1035		7
1605	Efficient evaluation of three-phase coexistence lines. 1994 , 15, 1073-1083		13
1604	Long-range contribution to inverse-distance power and Morse energy and pressure terms of a molecular liquid, tested on benzene. 1994 , 16, 61-71		
1603	Coexistence diagrams of mixtures by molecular simulation. 1994 , 49, 2633-2645		117
1602	A computational study of metastability in vapor-liquid equilibrium. 1994 , 49, 2717-2734		46
1601	Reaction field simulations of the vapor-liquid equilibria of dipolar fluids. 1994 , 231, 366-372		35

1600	Vapor-liquid equilibrium of a multipolar square-well fluid. 1994 , 202, 420-437		36
1599	Phase equilibria of binary Lennard-Jones mixtures: simulation and van der Waals l-fluid theory. <i>Fluid Phase Equilibria</i> , 1994 , 100, 153-170	2.5	50
1598	Equation of state calculations and Monte Carlo simulations of internal energies, compressibility factors and vapor-liquid equilibria for Lennard-Jones fluid mixtures. <i>Fluid Phase Equilibria</i> , 1994 , 95, 1-13	2.5	5
1597	Molecular simulation of liquid-liquid equilibria for Lennard-Jones fluids. <i>Fluid Phase Equilibria</i> , 1994 , 98, 129-139	2.5	23
1596	Numerical study of the phase diagram of a mixture of spherical and rodlike colloids. <i>Journal of Chemical Physics</i> , 1994 , 101, 9869-9875	3.9	99
1595	Determination of phase diagrams for the hard-core attractive Yukawa system. <i>Journal of Chemical Physics</i> , 1994 , 101, 4093-4097	3.9	383
1594	Coexisting phases and criticality in NaCl by computer simulation. <i>Journal of Chemical Physics</i> , 1994 , 101, 490-509	3.9	55
1593	A new algorithm for molecular dynamics simulations in the grand canonical ensemble. <i>Molecular Physics</i> , 1994 , 82, 439-453	1.7	12
1592	Reactive canonical Monte Carlo. <i>Molecular Physics</i> , 1994 , 81, 717-733	1.7	156
1591	Summary of the proceedings of the CALPHAD XXIII/AMSE 94 Meeting. 1994 , 18, 337-368		5
1590	Phase transitions in a continuum model of the classical Heisenberg magnet: The ferromagnetic system. 1994 , 49, 5169-5178		65
1589	Computer applications to materials science and engineering emphasized on the Japanese point of view. 1994 , 2, 103-110		
1588	Multibody distribution function contributions to the heat capacity for the truncated Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 1994 , 101, 7934-7938	3.9	5
1587	Free energy and phase equilibria for the restricted primitive model of ionic fluids from Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1994 , 101, 1452-1459	3.9	191
1586	Free energies and phase equilibria of chain molecules. 1994 , 81, 343-354		3
1585	Pore Size Distribution Analysis and Networking: Studies of Microporous Sorbents. 1994 , 51-60		21
1584	Monte Carlo Simulations of pVT Relations and Adsorption Equilibria of Ethane Under Sub- and Supercritical Conditions.. 1994 , 27, 228-234		4
1583	Phase transitions in thin films of symmetric binary polymer mixtures. <i>Molecular Physics</i> , 1994 , 81, 867-872	2.7	31

1582	Matrices are forever: On applied mathematics and computing in chemical engineering. 1995 , 50, 4005-4025		6
1581	An extension of the NpT plus test particle method for the determination of the vapour-liquid equilibria of pure fluids. 1995 , 235, 140-145		37
1580	A novel osmotic pressure route to the activity coefficient of a molecule in a solution. 1995 , 245, 178-182		15
1579	The NVT plus test particle method for the determination of the vapour-liquid equilibria of pure fluids. 1995 , 246, 214-220		23
1578	Monte carlo simulations of adsorption in a slitlike pore for binary mixtures of butane and carbon dioxide at supercritical conditions. <i>Fluid Phase Equilibria</i> , 1995 , 104, 305-316	2.5	18
1577	Structures and phase transitions in colloidal dispersions from theory and simulation. 1995 , 16, 327-335		8
1576	Phase equilibria in ternary Lennard-Jones systems. <i>Fluid Phase Equilibria</i> , 1995 , 107, 31-43	2.5	28
1575	Monte carlo simulations of phase coexistence for polymeric and ionic fluids. <i>Fluid Phase Equilibria</i> , 1995 , 104, 185-194	2.5	8
1574	Vapour liquid equilibria of Lennard-Jones model mixtures from the NpT plus test particle method. <i>Fluid Phase Equilibria</i> , 1995 , 112, 173-197	2.5	26
1573	Theoretical analysis of the far-infrared spectra of HCl in liquid Ar along the Ar liquid-vapour coexistence line. 1995 , 63, 251-264		4
1572	Phase diagram of a liquid crystal model: A computer simulation study. 1995 , 220, 113-138		42
1571	Monte Carlo simulations in the vicinity of the critical point: Vapour-liquid coexistence curve. 1995 , 45, 793-798		1
1570	Search of the liquid-vapor coexistence of the two-dimensional restricted primitive model. <i>Journal of Chemical Physics</i> , 1995 , 103, 4266-4272	3.9	3
1569	Parallel Gibbs-ensemble simulations. <i>Molecular Physics</i> , 1995 , 86, 171-183	1.7	17
1568	Simulating Complex Fluids. 1995 , 14, 259-274		11
1567	Gibbs-ensemble path-integral Monte Carlo simulations of a mixed quantum-classical fluid. 1995 , 51, 5162-5165		5
1566	Thermal relaxation of supercritical fluids by equilibrium molecular dynamics. 1995 , 51, 2013-2021		10
1565	Location of the Fisher-Widom line for systems interacting through short-ranged potentials. 1995 , 51, 3146-3155		26

1564	Computer simulation of vapor-liquid equilibria of linear dipolar fluids: Departures from the principle of corresponding states. <i>Journal of Chemical Physics</i> , 1995 , 102, 7204-7215	3.9	21
1563	Fluid-fluid phase separations in nonadditive hard sphere mixtures. <i>Journal of Chemical Physics</i> , 1995 , 102, 1349-1360	3.9	43
1562	Liquid-liquid phase equilibria of symmetrical mixtures by simulation in the semigrand canonical ensemble. <i>Journal of Chemical Physics</i> , 1995 , 103, 6188-6196	3.9	48
1561	Modified-hypernetted-chain determination of the phase diagram of rigid C60 molecules. 1995 , 51, 3387-3390		55
1560	Osmosis and reverse osmosis in solutions: Monte Carlo simulations and van der Waals one-fluid theory. <i>Molecular Physics</i> , 1995 , 86, 1473-1483	1.7	16
1559	Solid-liquid equilibrium for quadrupolar molecules. <i>Molecular Physics</i> , 1995 , 85, 413-421	1.7	15
1558	Microscopic theoretical determination of the phase diagram of the hard core Yukawa fluid. <i>Molecular Physics</i> , 1995 , 84, 125-131	1.7	20
1557	Phase-stability lines, spinodals and distribution functions for binary immiscible mixtures. <i>Molecular Physics</i> , 1995 , 86, 845-855	1.7	19
1556	Vapour liquid equilibria of mixtures from the NpT plus test particle method. <i>Molecular Physics</i> , 1995 , 85, 781-792	1.7	61
1555	Microstructure and phase behaviour of a mixed-dimer amphiphile. <i>Molecular Physics</i> , 1995 , 86, 201-223	1.7	5
1554	The condition of microscopic reversibility in Gibbs ensemble Monte Carlo simulations of phase equilibria. <i>Molecular Physics</i> , 1995 , 85, 435-447	1.7	20
1553	Can the Van der Waals loop vanish? II. Effect of domain size. <i>Molecular Physics</i> , 1995 , 84, 757-768	1.7	10
1552	Computer simulations of vapor-liquid phase equilibria of n-alkanes. <i>Journal of Chemical Physics</i> , 1995 , 102, 2126-2140	3.9	423
1551	Molecular Simulations of Thermodynamic Properties: From Argon to Long-Chain Paraffins. <i>Industrial & Engineering Chemistry Research</i> , 1995 , 34, 4166-4169	3.9	7
1550	Molecular simulation in a pseudo grand canonical ensemble. <i>Molecular Physics</i> , 1995 , 86, 139-147	1.7	30
1549	Vapour-liquid equilibria in two-dimensional Lennard-Jones fluids: unperturbed and substrate-mediated films. <i>Molecular Physics</i> , 1995 , 86, 599-612	1.7	41
1548	Thermodynamic and structural properties of model systems at solid-fluid coexistence. <i>Molecular Physics</i> , 1995 , 85, 43-59	1.7	250
1547	Molecular dynamics simulation of the orthobaric densities and surface tension of water. <i>Journal of Chemical Physics</i> , 1995 , 102, 4574-4583	3.9	557

1546	Finite-size scaling behavior of the free energy barrier between coexisting phases: Determination of the critical temperature and interfacial tension of the Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 1995 , 103, 8627-8637	3.9	56
1545	Fluid phase equilibria using molecular dynamics: the surface tension of chlorine and hexane. <i>Molecular Physics</i> , 1995 , 85, 651-663	1.7	51
1544	Solid-fluid coexistence for inverse-power potentials. 1995 , 74, 122-125		117
1543	Liquid-liquid phase transitions in pores. <i>Molecular Physics</i> , 1995 , 84, 825-834	1.7	44
1542	Stability of fluids with more than two components. <i>Molecular Physics</i> , 1995 , 84, 303-323	1.7	19
1541	Gelation of a clay colloid suspension. 1995 , 75, 2236-2239		169
1540	Vapour-liquid equilibria of propane and n-alkane conformers. <i>Molecular Physics</i> , 1995 , 85, 679-699	1.7	6
1539	Dielectric constant of a Stockmayer fluid along the vapour-liquid coexistence curve. <i>Molecular Physics</i> , 1995 , 85, 429-434	1.7	19
1538	Critical-point and coexistence-curve properties of the Lennard-Jones fluid: A finite-size scaling study. 1995 , 52, 602-611		385
1537	Monte Carlo simulations of phase equilibria for a lattice homopolymer model. <i>Journal of Chemical Physics</i> , 1995 , 102, 1014-1023	3.9	60
1536	Integral equation theory for uncharged liquids: The Lennard-Jones fluid and the bridge function. <i>Journal of Chemical Physics</i> , 1995 , 103, 2625-2633	3.9	104
1535	Simulations of reversible protein aggregate and crystal structure. 1996 , 70, 2888-902		49
1534	Simulation of Phase Equilibria for Lattice Polymers. 1996 , 29, 4066-4071		47
1533	Phase coexistence in a pseudo Gibbs ensemble. <i>Molecular Physics</i> , 1996 , 88, 1459-1469	1.7	23
1532	Effect of the attractive interactions on the phase behavior of the Gay-Berne liquid crystal model. <i>Journal of Chemical Physics</i> , 1996 , 105, 4234-4249	3.9	122
1531	Phase diagram for the Lennard-Jones fluid modelled by the hard-core Yukawa fluid. <i>Molecular Physics</i> , 1996 , 87, 1459-1462	1.7	16
1530	Gibbs-ensemble Monte Carlo simulation for the liquid-vapor coexistence of alkali fluids. 1996 , 205-207, 897-900		1
1529	Monte Carlo study of phase separation in aqueous protein solutions. <i>Journal of Chemical Physics</i> , 1996 , 104, 1646-1656	3.9	183

1528	Some Recent Developments in Computational Chemistry. 1996 , 16, 193-208		5
1527	Efficient pressure estimation in molecular simulations without evaluating the virial. <i>Journal of Chemical Physics</i> , 1996 , 105, 8469-8470	3.9	76
1526	Molecular simulation of the vapour-liquid equilibria of pure fluids and binary mixtures containing dipolar components: the effect of Keesom interactions. <i>Molecular Physics</i> , 1996 , 87, 979-990	1.7	27
1525	Expanded grand canonical and Gibbs ensemble Monte Carlo simulation of polymers. <i>Journal of Chemical Physics</i> , 1996 , 105, 4391-4394	3.9	181
1524	RESEARCH NOTE Molecular simulation of the liquid-liquid equilibria of binary mixtures containing dipolar and non-polar components interacting via the Keesom potential. <i>Molecular Physics</i> , 1996 , 89, 1187-1194	1.7	12
1523	Vapour-liquid equilibrium of Stockmayer fluids in applied field. <i>Molecular Physics</i> , 1996 , 87, 601-624	1.7	16
1522	Sensitivity Analysis of the Vapour-Liquid Phase Equilibria of a Model of Liquid Carbon Disulphide. 1996 , 194, 263-272		5
1521	Gibbs-Ensemble Molecular Dynamics: A New Method for Simulations Involving Particle Exchange. 1996 , 2, 319-326		9
1520	Integral equation theory description of phase equilibria in classical fluids. 1996 , 274, 1-105		220
1519	Molecular dynamics simulation of realistic systems. <i>Fluid Phase Equilibria</i> , 1996 , 116, 237-248	2.5	6
1518	Current advances in Monte Carlo methods. <i>Fluid Phase Equilibria</i> , 1996 , 116, 257-266	2.5	27
1517	Alternative implementations of the Gibbs ensemble Monte Carlo calculation. 1996 , 261, 620-624		24
1516	Vapor-liquid equilibria of binary mixtures containing methane, ethane, and carbon dioxide from molecular simulation. 1996 , 17, 889-908		35
1515	Phase transitions and quantum effects in adsorbed monolayers. 1996 , 17, 157-167		11
1514	Monte Carlo simulation of fluid phase equilibria in pore systems: square-well fluid distributed over a bulk and a slit-pore. 1996 , 249, 470-475		11
1513	A new simulation method for the determination of the vapour-liquid equilibria in the grand canonical ensemble. 1996 , 256, 474-482		16
1512	Calculation of thermodynamic derivatives from NPT computer simulation in combination with the Kirkwood-Buff theory. 1996 , 258, 271-275		5
1511	Molecular simulations of fluid phase equilibria. <i>Fluid Phase Equilibria</i> , 1996 , 116, 249-256	2.5	6

1510	Simulation of chain molecules for prediction of thermodynamic properties. <i>Fluid Phase Equilibria</i> , 1996 , 116, 312-319	2.5	2
1509	Vapour-liquid and liquid-liquid phase equilibria of binary mixtures containing helium: comparison of experiment with predictions using equations of state. <i>Fluid Phase Equilibria</i> , 1996 , 122, 1-15	2.5	19
1508	Towards a theory of coexistence and criticality in real molten salts. <i>Molecular Physics</i> , 1996 , 87, 37-86	1.7	43
1507	An Improved First-Order Perturbation Theory of Simple Fluids Using High Temperature Approximation and Random Phase Approximation. 1996 , 33, 17-36		
1506	Prediction of the vapour-liquid coexistence curve of alkanols by molecular simulation. <i>Molecular Physics</i> , 1996 , 87, 87-101	1.7	34
1505	The isotropic-nematic phase transition in uniaxial hard ellipsoid fluids: Coexistence data and the approach to the Onsager limit. <i>Journal of Chemical Physics</i> , 1996 , 105, 2837-2849	3.9	106
1504	Phase diagram of the two-dimensional Coulomb gas: A thermodynamic scaling Monte Carlo study. <i>Journal of Chemical Physics</i> , 1996 , 104, 7205-7209	3.9	31
1503	On the equilibrium and time relaxation of a lattice gas in several boxes. <i>Molecular Physics</i> , 1996 , 88, 1157-1171	3.9	112
1502	Absence of criticality in the reference hypernetted chain equation for short ranged potentials. <i>Molecular Physics</i> , 1996 , 87, 1235-1242	1.7	5
1501	Vapour-liquid equilibria of exponential-six fluids. <i>Molecular Physics</i> , 1996 , 87, 1471-1476	1.7	10
1500	Reference hypernetted chain theory for linear molecular fluids: A comprehensive study of the gas-liquid coexistence. <i>Journal of Chemical Physics</i> , 1996 , 105, 4265-4273	3.9	6
1499	Towards the atomistic simulation of phase coexistence in nonequilibrium systems. <i>Journal of Chemical Physics</i> , 1996 , 105, 2378-2390	3.9	6
1498	Island of vapor-liquid coexistence in dipolar hard-core systems. 1996 , 76, 4183-4186		61
1497	Phase behavior of the Widom-Bowlinson mixture. <i>Journal of Chemical Physics</i> , 1996 , 104, 7665-7670	3.9	28
1496	Liquid-liquid equilibrium for fluids confined within random porous materials. <i>Journal of Chemical Physics</i> , 1996 , 105, 4257-4264	3.9	43
1495	Phase equilibria of a lattice model for an oil-water-amphiphile mixture. <i>Journal of Chemical Physics</i> , 1996 , 104, 3718-3725	3.9	50
1494	An efficient approach to estimating thermodynamic properties of fluid mixtures in molecular simulation. <i>Journal of Chemical Physics</i> , 1996 , 104, 3709-3717	3.9	4
1493	Simulation and prediction of vapour-liquid equilibria for chain molecules. <i>Molecular Physics</i> , 1996 , 87, 347-366	1.7	77

1492	On the phase diagrams of fluids of linearly fused Lennard-Jones sites. <i>Molecular Physics</i> , 1996 , 88, 543-557		4
1491	Gibbs-Ensemble Molecular Dynamics: Liquid-Gas Equilibria for Lennard-Jones Spheres and n-Hexane. 1996 , 17, 95-112		16
1490	Monte Carlo Simulation Study of Adsorption Characteristics in Slit-Like Micropores Under Supercritical Conditions. 1996 , 16, 291-305		13
1489	Understanding the critical properties of chain molecules. <i>Molecular Physics</i> , 1996 , 88, 1575-1602	1.7	20
1488	On the Molecular Dynamics Algorithm for Gibbs Ensemble Simulation. 1996 , 17, 21-25		14
1487	Computational physics in petrochemical industry. 1996 , T66, 80-84		5
1486	Computer Simulations of Water between Hydrophobic Surfaces: The Hydrophobic Force. 1996 , 100, 15005-15010		41
1485	The vapour - liquid equilibrium of n-alkanes. <i>Journal of Physics Condensed Matter</i> , 1996 , 8, 9643-9648	1.8	3
1484	Vapour - liquid equilibria of binary mixtures containing Stockmayer molecules. <i>Journal of Physics Condensed Matter</i> , 1997 , 9, 3349-3360	1.8	10
1483	Path-integral Monte Carlo simulations of a supercritical fluid. 1997 , 56, 13927-13931		6
1482	Finite-size critical behavior in the Gibbs ensemble. 1997 , 55, 2315-2320		11
1481	Influence of three-body forces on the gas-liquid coexistence of simple fluids: The phase equilibrium of argon. 1997 , 55, 2707-2712		57
1480	Numerical study of the phase behavior of rodlike colloids with attractive interactions. <i>Journal of Chemical Physics</i> , 1997 , 107, 1551-1564	3.9	150
1479	Path integral grand canonical Monte Carlo. <i>Journal of Chemical Physics</i> , 1997 , 107, 5108-5117	3.9	84
1478	Statistical model for the structure and gelation of smectite clay suspensions. 1997 , 55, 3044-3053		116
1477	Thermodynamic behaviour of homonuclear and heteronuclear Lennard-Jones chains with association sites from simulation and theory. <i>Molecular Physics</i> , 1997 , 92, 135-150	1.7	184
1476	Improving the Efficiency of a New Infinite Order Perturbation Method to Simulate Surface Forces. 1997 , 19, 85-91		9
1475	Vapor-liquid coexistence of quasi-two-dimensional Stockmayer fluids. <i>Journal of Chemical Physics</i> , 1997 , 106, 3311-3317	3.9	49

1474	Pseudo-ensemble simulations and Gibbs-Duhem integrations for polymers. <i>Journal of Chemical Physics</i> , 1997 , 106, 2911-2923	3.9	28
1473	Novel procedure to determine coexistence lines by computer simulation. Application to hard-core Yukawa model for charge-stabilized colloids. <i>Journal of Chemical Physics</i> , 1997 , 106, 4678-4683	3.9	58
1472	Critical behavior of the square-well fluid with ϵ_2 : A finite-size-scaling study. 1997 , 55, 1347-1354		41
1471	Phase transitions of quadrupolar fluids. <i>Journal of Chemical Physics</i> , 1997 , 107, 237-242	3.9	11
1470	Influence of association on the liquid-vapor phase coexistence of simple systems. <i>Journal of Chemical Physics</i> , 1997 , 106, 1569-1575	3.9	11
1469	Local free energy calculations in simulations. <i>Journal of Chemical Physics</i> , 1997 , 106, 2771-2776	3.9	5
1468	Phase coexistence properties of polarizable Stockmayer fluids. <i>Journal of Chemical Physics</i> , 1997 , 106, 3338-3347	3.9	53
1467	Monte Carlo simulation of athermal mesogenic chains: Pure systems, mixtures, and constrained environments. <i>Journal of Chemical Physics</i> , 1997 , 106, 9858-9868	3.9	61
1466	The role of local density in the collisional deactivation of vibrationally highly excited azulene in supercritical fluids. <i>Journal of Chemical Physics</i> , 1997 , 107, 8380-8390	3.9	96
1465	A Gibbs ensemble Monte Carlo study of phase coexistence in model C60. <i>Journal of Chemical Physics</i> , 1997 , 106, 255-263	3.9	57
1464	Molecular dynamics study of liquid CH ₂ F ₂ (HFC-32). <i>Molecular Physics</i> , 1997 , 92, 641-650	1.7	12
1463	Monte Carlo simulations of racemic liquid mixtures: thermodynamic properties and local structure. <i>Molecular Physics</i> , 1997 , 91, 19-30	1.7	22
1462	Chapter 15. Structure of porous adsorbents: Analysis using density functional theory and molecular simulation. 1997 , 104, 745-775		46
1461	Multiphase equilibria using the Gibbs ensemble Monte Carlo method. <i>Molecular Physics</i> , 1997 , 92, 187-196		36
1460	Tracing the phase boundaries of hard spherocylinders. <i>Journal of Chemical Physics</i> , 1997 , 106, 666-687	3.9	624
1459	De Gruyter. 1997 , 199, 61-68		5
1458	Determination of vapour-liquid equilibrium using cavity-biased grand canonical Monte Carlo method. <i>Molecular Physics</i> , 1997 , 92, 1067-1072	1.7	18
1457	Application of a new Gibbs ensemble Monte Carlo method to site-site interaction model fluids. <i>Molecular Physics</i> , 1997 , 90, 1031-1034	1.7	11

1456	Density Functional Theory for Studies of Multiple States of Inhomogeneous Fluids at Solid Surfaces and in Pores. 1997 , 492, 27		2
1455	Monte Carlo Simulations of Fluid Phase Transitions in Micropores: Hysteresis and Van Der Waals-Type Loops. 1997 , 492, 35		
1454	Simulations of phase equilibria in planar slits. <i>Molecular Physics</i> , 1997 , 90, 637-652	1.7	8
1453	Lattice Theories and Simulation Studies of Polymer Solutions on BCC and FCC Lattices. 1997 , 30, 5096-5103		2
1452	Intermolecular potentials for branched alkanes and the vapour-liquid phase equilibria of n-heptane, 2-methylhexane, and 3-ethylpentane. <i>Molecular Physics</i> , 1997 , 90, 687-694	1.7	42
1451	Can osmotic pressure be negative?. <i>Molecular Physics</i> , 1997 , 90, 665-670	1.7	7
1450	Determination of adsorption equilibria in pores by molecular dynamics in a unit cell with imaginary gas phase. <i>Journal of Chemical Physics</i> , 1997 , 106, 8124-8134	3.9	52
1449	Quantitative comparison and optimization of methods for evaluating the chemical potential by molecular simulation. <i>Molecular Physics</i> , 1997 , 92, 973-996	1.7	162
1448	Gibbs-Duhem integration in lattice systems. 1997 , 40, 111-116		5
1447	Predicting Multicomponent Phase Equilibria and Free Energies of Transfer for Alkanes by Molecular Simulation. 1997 , 119, 8921-8924		143
1446	Molecular Simulation of Henry's Constant at Vapor-Liquid and Liquid-Liquid Phase Boundaries. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 3834-3838	3.4	16
1445	Gas-Liquid Coexistence Properties from Reference Hypernetted Chain Theory for Linear Polar Solvents. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 1451-1459	3.4	6
1444	Monte Carlo Simulations of Liquid-Liquid Equilibria for Ternary Chain Molecule Systems on a Lattice. 1997 , 30, 8459-8462		13
1443	Thermodynamics of Chain Fluids from Atomistic Simulation: A Test of the Chain Increment Method for Chemical Potential. 1997 , 30, 4744-4755		41
1442	Statistical associating fluid theory for chain molecules with attractive potentials of variable range. <i>Journal of Chemical Physics</i> , 1997 , 106, 4168-4186	3.9	864
1441	The dependence of the phase diagram on the range of the attractive intermolecular forces. <i>Journal of Physics Condensed Matter</i> , 1997 , 9, 3361-3370	1.8	43
1440	Applications of Monte Carlo methods to statistical physics. 1997 , 60, 487-559		469
1439	Effective Intermolecular Potential for Fluid Hydrogen Sulfide. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 5480-5483	3.4	92

- ¹⁴³⁸ Dynamical properties and transport coefficients of Kihara linear fluids. *Journal of Chemical Physics*, **1997**, 106, 4753-4767 3.9 12
- ¹⁴³⁷ Vapour-Liquid Phase Equilibria Predictions of Methane-Alkane Mixtures by Monte Carlo Simulation. **1997**, 19, 1-15 76
- ¹⁴³⁶ Phase transitions in nonadditive hard disc systems: a Gibbs ensemble Monte Carlo Study. **1997**, 166-167
- ¹⁴³⁵ Properties of coexisting fluid phases of a binary system methanol-ethane by computer simulation. *Fluid Phase Equilibria*, **1997**, 129, 1-13 2.5 12
- ¹⁴³⁴ Calculation of chemical potential for structured molecules using osmotic molecular dynamics simulations. *Fluid Phase Equilibria*, **1997**, 137, 75-85 2.5 7
- ¹⁴³³ Computer modeling and simulation of geofluids: A general review and sample description. **1997**, 16, 240-247
- ¹⁴³² Determination of the micropore volume distribution function of activated carbons by gas adsorption. **1997**, 3, 55-65 5
- ¹⁴³¹ Gibbs Ensemble Monte Carlo simulation of binary vapor-liquid equilibria for CFC alternatives. *Fluid Phase Equilibria*, **1997**, 130, 157-166 2.5 8
- ¹⁴³⁰ Molecular simulation of the vapor-liquid equilibrium of methanethiol + propane mixtures. *Fluid Phase Equilibria*, **1997**, 131, 51-65 2.5 8
- ¹⁴²⁹ Phase equilibrium of quantum fluids from simulation: Hydrogen and neon. *Fluid Phase Equilibria*, **1997**, 132, 93-116 2.5 59
- ¹⁴²⁸ Exploration of the vapour-liquid phase equilibria and critical points of triacontane isomers. *Fluid Phase Equilibria*, **1997**, 134, 55-61 2.5 32
- ¹⁴²⁷ Molecular simulation of intermolecular attraction and repulsion in coexisting liquid and vapour phases. *Fluid Phase Equilibria*, **1997**, 134, 77-85 2.5 13
- ¹⁴²⁶ Analytical equation of state based on the Ornstein-Zernike equation. *Fluid Phase Equilibria*, **1997**, 134, 21-42 2.5 87
- ¹⁴²⁵ Vapor-liquid equilibria for pure substances by Gibbs ensemble simulation of Stockmayer potential molecules. *Fluid Phase Equilibria*, **1997**, 137, 87-98 2.5 10
- ¹⁴²⁴ Phase separations for mixtures in well-characterized porous materials: Liquid-liquid transitions. *Fluid Phase Equilibria*, **1997**, 136, 93-109 2.5 21
- ¹⁴²³ Configurational bias Gibbs ensemble Monte Carlo simulation of vapor-liquid equilibria of linear and short-branched alkanes. *Fluid Phase Equilibria*, **1997**, 141, 45-61 2.5 37
- ¹⁴²² Monte Carlo simulation of the nematic-vapour interface for a Gay-Berne liquid crystal. **1997**, 271, 241-246 29
- ¹⁴²¹ Polymer chain collapse near the lower critical solution temperature. **1997**, 278, 302-306 40

1420	Effect of the shape of simulation box on the Van der Waals loop of a Lennard-Jones fluid. 1998 , 282, 128-132		2
1419	Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture. <i>Journal of Chemical Physics</i> , 1998 , 109, 10914-10920	3.9	313
1418	Vapor-liquid equilibria from molecular simulations using the algorithm in equation of state calculations. <i>Fluid Phase Equilibria</i> , 1998 , 144, 137-144	2.5	4
1417	Combining Dissipative Particle Dynamics and Monte Carlo Techniques. 1998 , 147, 507-517		24
1416	Solvation effect on kinetic rate constant of reactions in supercritical solvents. 1998 , 44, 667-680		33
1415	Recent contributions of statistical mechanics in chemical engineering. 1998 , 44, 2569-2596		24
1414	Molecular dynamic simulation and equation of state of Lennard-Jones chain fluids. 1998 , 15, 544-551		8
1413	Molecular dynamics methodology for the study of the solvent effects on a concentrated Diels-Alder reaction and the separation of the post-reaction mixture. 1998 , 22, S27-S33		8
1412	Numerical simulations of solvation in simple polar fluids: dependence on the thermodynamic state below and above the critical point. 1998 , 235, 297-312		24
1411	Intermolecular potentials and vapor-liquid phase equilibria of perfluorinated alkanes. <i>Fluid Phase Equilibria</i> , 1998 , 146, 51-61	2.5	84
1410	Monte Carlo simulation of high-pressure phase equilibria in aqueous systems. <i>Fluid Phase Equilibria</i> , 1998 , 150-151, 33-40	2.5	22
1409	Classical molecular simulations of complex, industrially-important systems on the intel paragon. 1998 , 35, 73-84		3
1408	Understanding the phase diagrams of quadrupolar molecules. 1998 , 76, 157-169		8
1407	On the simulation of vapor-liquid equilibria for alkanes. <i>Journal of Chemical Physics</i> , 1998 , 108, 9905-9913	3.9	378
1406	Phase equilibria of the modified Buckingham exponential-6 potential from Hamiltonian scaling grand canonical Monte Carlo. <i>Journal of Chemical Physics</i> , 1998 , 109, 1093-1100	3.9	89
1405	Thermodynamic Properties of the Williams, OPLS-AA, and MMFF94 All-Atom Force Fields for Normal Alkanes. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 2578-2586	3.4	81
1404	Variational perturbation calculations for the phase diagram of systems with short-ranged interactions. <i>Journal of Chemical Physics</i> , 1998 , 108, 208-217	3.9	42
1403	The thermodynamics of mixtures and the corresponding mixing rules in the SAFT-VR approach for potentials of variable range. <i>Molecular Physics</i> , 1998 , 93, 241-252	1.7	195

1402	Molecular Simulation of the Pure n-Hexadecane Vapor-Liquid Equilibria at Elevated Temperature. 1998 , 31, 1430-1431		9
1401	Alternative Gibbs ensemble Monte Carlo implementations: application in mixtures. <i>Molecular Physics</i> , 1998 , 94, 519-525	1.7	7
1400	Liquid-vapor phase behavior of a symmetrical binary fluid mixture. 1998 , 58, 2201-2212		106
1399	A Fixed Point Charge Model for Water Optimized to the Vapor-Liquid Coexistence Properties. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 7470-7475	3.4	167
1398	Simulation of Vapor-Liquid Equilibria for Alkane Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 3195-3202	3.9	43
1397	Computer simulation study of gas-liquid nucleation in a Lennard-Jones system. <i>Journal of Chemical Physics</i> , 1998 , 109, 9901-9918	3.9	389
1396	Prediction of Binary and Ternary Diagrams Using the Statistical Associating Fluid Theory (SAFT) Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 660-674	3.9	219
1395	Molecular Simulation of Phase Equilibria for Water-Methane and Water-Ethane Mixtures. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 8865-8873	3.4	108
1394	Application of polyelectrolyte theories for analysis of DNA melting in the presence of Na ⁺ and Mg ²⁺ ions. 1998 , 75, 3041-56		50
1393	Transferable Potentials for Phase Equilibria. 1. United-Atom Description of n-Alkanes. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 2569-2577	3.4	2075
1392	Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 1029-1035	3.4	148
1391	Vapor-Liquid Equilibria of Binary and Ternary Mixtures Containing Methane, Ethane, and Carbon Dioxide from Gibbs Ensemble Simulations. <i>Journal of Physical Chemistry B</i> , 1998 , 102, 7627-7631	3.4	25
1390	Restricted primitive model of an ionic solution confined to a plane. <i>Journal of Chemical Physics</i> , 1998 , 109, 7486-7497	3.9	25
1389	Novel pseudoensembles for simulation of multicomponent phase equilibria. <i>Journal of Chemical Physics</i> , 1998 , 108, 8761-8772	3.9	62
1388	Vapor-Liquid equilibria and heat effects of hydrogen fluoride from molecular simulation. <i>Journal of Chemical Physics</i> , 1998 , 109, 4015-4027	3.9	23
1387	A comprehensive study of the phase diagram of symmetrical hard-core Yukawa mixtures. <i>Journal of Chemical Physics</i> , 1998 , 109, 4498-4507	3.9	24
1386	Solid-Liquid equilibrium for a molecular model with short ranged directional forces. <i>Journal of Chemical Physics</i> , 1998 , 109, 9938-9949	3.9	67
1385	Preroughening, fractional-layer occupancies, and phase separation at a disordered flat metal surface. 1998 , 57, 10157-10165		5

- 1384 Critical-point of the Lennard-Jones fluid: A finite-size scaling study. *Journal of Chemical Physics*, **1998**, 109, 4885-4893 3.9 68
- 1383 Gas-liquid coexistence and demixing in systems with highly directional pair potentials. **1998**, 57, 5682-5686 26
- 1382 Phase behavior of nonadditive hard-sphere mixtures. **1998**, 58, 7523-7528 47
- 1381 Phase Equilibria of Mixtures Containing Chain Molecules Predicted through a Novel Simulation Scheme. **1998**, 80, 4466-4469 49
- 1380 Phase equilibria of a square-well monomer-dimer mixture: Gibbs ensemble computer simulation and statistical associating fluid theory for potentials of variable range. **1998**, 57, 2035-2044 17
- 1379 Calculation of solid-fluid phase equilibria for systems of chain molecules. *Journal of Chemical Physics*, **1998**, 109, 318-328 3.9 42
- 1378 Molecular-dynamics study of the Girifalco-model C60 at two high-temperature isotherms. **1998**, 58, 2372-2375 11
- 1377 Outside and inside the critical region of the Lennard-Jones fluid. *Journal of Chemical Physics*, **1998**, 109, 5935-5944 3.9 54
- 1376 Thermodynamic scaling Monte Carlo study of the liquid-gas transition in the square-well fluid. *Journal of Chemical Physics*, **1998**, 108, 1115-1122 3.9 24
- 1375 Simulations of Carbon Containing Semiconductor Alloys: Bonding, Strain Compensation, and Surface Structure. **1998**, 09, 357-389 32
- 1374 Monte Carlo simulation of some thermophysical properties of two-centre Lennard-Jones fluids along the vapour-liquid equilibrium curve. *Molecular Physics*, **1998**, 93, 279-286 1.7 3
- 1373 . *Advances in Chemical Physics*, **1999**, 1 1
- 1372 Tracing coexistence lines in multicomponent fluid mixtures by molecular simulation. *Journal of Chemical Physics*, **1999**, 110, 11999-12010 3.9 32
- 1371 Simulation Study of the Link between Molecular Association and Reentrant Miscibility for a Mixture of Molecules with Directional Interactions. **1999**, 82, 5285-5288 24
- 1370 Comment on Gas-liquid coexistence and demixing in systems with highly directional pair potentials **1999**, 59, 1280-1282 1
- 1369 Simulation of swelling of model polymeric gels by subcritical and supercritical solvents. *Journal of Chemical Physics*, **1999**, 110, 1290-1298 3.9 19
- 1368 Phase diagram of the four-dimensional Lennard-Jones fluid. *Journal of Chemical Physics*, **1999**, 111, 8043-8047 3.9 6
- 1367 Molecular Simulation of Vapour-Liquid Coexistence Curves for Hydrogen Sulfide-Alkane and Carbon Dioxide-Alkane Mixtures. **1999**, 22, 351-368 26

1366	Strict detailed balance is unnecessary in Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 1999 , 110, 2753-2756	3.9	123
1365	Vapour-liquid coexistence curves of the united-atom and anisotropic united-atom force fields for alkane mixtures. <i>Molecular Physics</i> , 1999 , 96, 1517-1524	1.7	31
1364	Determination of potential parameters for alkanes. <i>Journal of Chemical Physics</i> , 1999 , 111, 438-439	3.9	11
1363	Nematic-isotropic transition in polydisperse systems of infinitely thin hard platelets. <i>Journal of Chemical Physics</i> , 1999 , 110, 6553-6559	3.9	135
1362	A biased grand canonical Monte Carlo method for simulating adsorption using all-atom and branched united atom models. <i>Molecular Physics</i> , 1999 , 96, 1375-1390	1.7	141
1361	Direct calculation of bubble points by Monte Carlo simulation. <i>Molecular Physics</i> , 1999 , 97, 523-539	1.7	29
1360	Molecular dynamics simulation of the liquid-vapor interface: Binary mixtures of Lennard-Jones fluids. <i>Journal of Chemical Physics</i> , 1999 , 110, 1188-1194	3.9	77
1359	Free energy calculations on systems of rigid molecules: An application to the TIP4P model of H ₂ O. <i>Journal of Chemical Physics</i> , 1999 , 110, 55-61	3.9	86
1358	Derivation of a general fluid equation of state based on the quasi-Gaussian entropy theory: application to the Lennard-Jones fluid. <i>Molecular Physics</i> , 1999 , 96, 1469-1490	1.7	15
1357	Computer simulation study of liquid CH ₂ F ₂ with a new effective pair potential model. <i>Journal of Chemical Physics</i> , 1999 , 110, 2991-3002	3.9	25
1356	Asymmetric growth in micelles containing oil. <i>Journal of Chemical Physics</i> , 1999 , 110, 9673-9680	3.9	17
1355	SIMULATION OF NEMATIC FREE SURFACES. 1999 , 10, 431-443		7
1354	The Boundary Condition in the Gibbs Ensemble Simulation of a Stockmayer Fluid under an Applied Field. 1999 , 23, 95-107		9
1353	Molecular simulations on volumetric properties of natural gas. <i>Fluid Phase Equilibria</i> , 1999 , 161, 45-62	2.5	16
1352	A comparison of molecular-based models to determine vapor-liquid phase coexistence in hydrogen fluoride. <i>Fluid Phase Equilibria</i> , 1999 , 158-160, 37-47	2.5	25
1351	Gibbs ensemble simulation of HCFC/HFC mixtures by effective Stockmayer potential. <i>Fluid Phase Equilibria</i> , 1999 , 158-160, 69-78	2.5	20
1350	Strong weak and metastable liquids structural and dynamical aspects of the liquid state. 1999 , 263, 378-388		82
1349	Monte Carlo simulations of squalane in the Gibbs ensemble. <i>Fluid Phase Equilibria</i> , 1999 , 155, 167-176	2.5	15

1348	Molecular simulation with an EOS algorithm for vapor-liquid equilibria of oxygen and ethane. <i>Fluid Phase Equilibria</i> , 1999 , 158-160, 29-35	2.5	11
1347	Crossover Flory model for phase separation in polymer solutions. 1999 , 264, 345-369		44
1346	Gibbs ensemble computer simulation and SAFT-VR theory of non-conformal square-well monomer-dimer mixtures. 1999 , 303, 27-36		22
1345	Simulation of phase transitions in fluids. 1999 , 50, 377-411		87
1344	Evaluation of a locus of azeotropes by molecular simulation. 1999 , 45, 2237-2244		11
1343	Critical properties of mixtures of alkanes from perturbation theory. <i>Journal of Chemical Physics</i> , 1999 , 111, 3183-3191	3.9	8
1342	Solubility of Small Molecules and Their Mixtures in Polyethylene. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 3539-3544	3.4	37
1341	Monte Carlo approach to the gas-liquid transition in porous materials. 1999 , 60, 5495-504		68
1340	Effect of uniform electric field on homogeneous vapor-liquid nucleation and phase equilibria. II. Extended simple point charge model water. <i>Journal of Chemical Physics</i> , 1999 , 110, 2533-2538	3.9	31
1339	Simulating Retention in Gas-Liquid Chromatography. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 11191-11195	3.9	23
1338	Vapor-Liquid Phase Coexistence of Alkane-Carbon Dioxide and Perfluoroalkane-Carbon Dioxide Mixtures. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 4485-4491	3.4	58
1337	Calculation of the vapour-liquid coexistence curve for a fluctuating point charge water model. <i>Molecular Physics</i> , 1999 , 97, 993-996	1.7	22
1336	Micellization in Model Surfactant Systems. 1999 , 15, 3143-3151		179
1335	Numerical prediction of the melting curve of n-octane. <i>Journal of Chemical Physics</i> , 1999 , 111, 1501-1510	3.9	47
1334	A New Intermolecular Potential Model for the n-Alkane Homologous Series. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 6314-6322	3.4	162
1333	Constant pressure Gibbs ensemble Monte Carlo simulations of adsorption into narrow pores. <i>Molecular Physics</i> , 1999 , 97, 955-965	1.7	63
1332	Gibbs ensemble simulations of vapour-liquid phase equilibria of cyclic alkanes. <i>Molecular Physics</i> , 1999 , 97, 769-776	1.7	25
1331	Computer simulations of liquid/vapor interface in Lennard-Jones fluids: Some questions and answers. <i>Journal of Chemical Physics</i> , 1999 , 111, 8510-8523	3.9	383

1330	Novel Configurational-Bias Monte Carlo Method for Branched Molecules. Transferable Potentials for Phase Equilibria. 2. United-Atom Description of Branched Alkanes. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 4508-4517	3.4	707
1329	Phase separation in confined systems. 1999 , 62, 1573-1659		1349
1328	Transferable Potentials for Phase Equilibria. 3. Explicit-Hydrogen Description of Normal Alkanes. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 5370-5379	3.4	233
1327	Phase equilibria in binary Lennard-Jones mixtures: phase diagram simulation. <i>Molecular Physics</i> , 1999 , 96, 1649-1658	1.7	18
1326	Molecular simulation of phase equilibria for mixtures of polar and non-polar components. <i>Molecular Physics</i> , 1999 , 97, 1073-1083	1.7	126
1325	Molecular Simulation of Olefins Using a New United-Atom Potential Model: Vapor-Liquid Equilibria of Pure Compounds and Mixtures. 1999 , 121, 3407-3413		26
1324	Origins of the Solvent Chain-Length Dependence of Gibbs Free Energies of Transfer. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 2977-2980	3.4	13
1323	Accurate Computer Simulation of Phase Equilibrium for Complex Fluid Mixtures. Application to Binaries Involving Isobutene, Methanol, Methyl tert-Butyl Ether, and n-Butane. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 10496-10505	3.4	34
1322	Solid-Liquid phase equilibrium for binary Lennard-Jones mixtures. <i>Journal of Chemical Physics</i> , 1999 , 110, 11433-11444	3.9	70
1321	A simple effective pair potential for the molecular simulation of the thermodynamic properties of ammonia. <i>Molecular Physics</i> , 1999 , 97, 1129-1137	1.7	47
1320	Exploring Multicomponent Phase Equilibria by Monte Carlo Simulations: Toward a Description of Gas-Liquid Chromatography. 1999 , 82-95		4
1319	Computer Simulation of Fractionation in Bidisperse Liquid Crystals. 1999 , 330, 423-430		1
1318	Thermodynamic Integration Along Coexistence Lines. 1999 , 7, 99-127		2
1317	Some aspects of the Methodology in Gibbs Ensemble Monte Carlo Simulations in Connection with a Model Fluid of C60. 1999 , 21, 227-238		
1316	An Extended Gibbs Ensemble. 1999 , 22, 183-198		8
1315	Molecular and macroscopic modeling of phase separation. 2000 , 46, 2086-2096		13
1314	A simple molecular dynamics simulation for calculating Henry's constant and solubility of gases in liquids. 2000 , 319, 60-64		25
1313	Computer simulation of the interface between two liquid crystalline phases in rod-plate binary mixtures. 2000 , 325, 631-638		22

1312	A multiple chain Monte Carlo method for atomistic simulation of high molecular weight polymer melts. 2000 , 10, 29-41		3
1311	Long-range behaviour in liquid crystals by computer simulation. 2000 , 85, 161-171		1
1310	Extension of the NpT + test particle method for the calculation of phase equilibria of nitrogen + ethane. 2000 , 85, 237-247		14
1309	Vapor+liquid equilibrium of water, carbon dioxide, and the binary system, water+carbon dioxide, from molecular simulation. <i>Fluid Phase Equilibria</i> , 2000 , 170, 203-234	2.5	125
1308	Predicting Solvent Effects on Reactions and Liquid-Liquid Equilibrium by Computer Simulation. 2000 , 78, 1077-1083		3
1307	Monte Carlo simulation of thermodynamic properties for two-dimensional Lennard-Jones fluids. 2000 , 45, 2004-2009		8
1306	Parallelized sampling of the Gibbs ensemble. <i>Molecular Physics</i> , 2000 , 98, 1887-1894	1.7	3
1305	Molecular Simulation and Modeling of Supercritical Water and Aqueous Solutions. 2000 , 345-394		
1304	6 Equations of state from analytically solvable integral equation approximations. 2000 , 169-254		5
1303	Depletion and bridging forces in polymer systems: Monte Carlo simulations at constant chemical potential. <i>Journal of Chemical Physics</i> , 2000 , 113, 5493	3.9	29
1302	Computer simulation of acetonitrile and methanol with ab initio-based pair potentials. <i>Journal of Chemical Physics</i> , 2000 , 113, 5401	3.9	26
1301	Computer simulation of the chemical potential of binary Lennard-Jones mixtures. <i>Journal of Chemical Physics</i> , 2000 , 112, 2315-2318	3.9	6
1300	Gibbs ensemble simulation of water in spherical cavities. <i>Journal of Chemical Physics</i> , 2000 , 113, 5026	3.9	60
1299	Line of triple points for the hard-core Yukawa model: A computer simulation study. <i>Journal of Chemical Physics</i> , 2000 , 112, 5121-5126	3.9	51
1298	Can the visual molecular configuration in computer simulations locate solid-liquid phase boundaries? The case of C60. <i>Journal of Chemical Physics</i> , 2000 , 113, 4315-4319	3.9	20
1297	Liquid-vapor coexistence by molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 2000 , 112, 3516-3522	3.5	2
1296	Temperature and density extrapolations in canonical ensemble monte carlo simulations. 2000 , 61, 1195-8		5
1295	Closed-loop phase equilibria of a symmetrical associating mixture of square-well molecules examined by Gibbs ensemble Monte Carlo simulation. 2000 , 61, 2245-2256		13

1294	Phase equilibria and thermodynamic properties of hard core Yukawa fluids of variable range from simulations and an analytical theory. <i>Journal of Chemical Physics</i> , 2000 , 112, 10358-10367	3.9	85
1293	Simulation and extrapolation of coexistence properties with single-phase and two-phase ensembles. <i>Journal of Chemical Physics</i> , 2000 , 113, 8444-8456	3.9	20
1292	Interaction between solute molecules in medium density solvents. <i>Molecular Physics</i> , 2000 , 98, 725-736	1.7	6
1291	Monte Carlo methods for phase equilibria of fluids. <i>Journal of Physics Condensed Matter</i> , 2000 , 12, R25-R58	1.8	210
1290	Transferable Potentials for Phase Equilibria. 4. United-Atom Description of Linear and Branched Alkenes and Alkylbenzenes. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 8008-8016	3.4	435
1289	The Chemical Meaning of the Standard Free Energy of Transfer: Use of van der Waals' Equation of State To Unravel the Interplay between Free Volume, Volume Entropy, and the Role of Standard States. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 5343-5349	3.4	27
1288	Liquid-vapor coexistence curves of several interatomic model potentials. <i>Journal of Chemical Physics</i> , 2000 , 113, 9162-9168	3.9	124
1287	Adiabatic Nuclear and Electronic Sampling Monte Carlo Simulations in the Gibbs Ensemble: Application to Polarizable Force Fields for Water. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 2378-2390	3.4	66
1286	Gauge cell method for simulation studies of phase transitions in confined systems. 2000 , 62, 4611-22		132
1285	Force Field of Monoethanolamine. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 1332-1337	3.4	83
1284	Optimization of the anisotropic united atoms intermolecular potential for n-alkanes. <i>Journal of Chemical Physics</i> , 2000 , 112, 5499-5510	3.9	252
1283	Predicting the gas-liquid critical point from the second virial coefficient. <i>Journal of Chemical Physics</i> , 2000 , 112, 5364-5369	3.9	211
1282	Molecular dynamics simulation of supersaturated vapor nucleation in slit pore. <i>Journal of Chemical Physics</i> , 2000 , 112, 4279-4285	3.9	48
1281	Self-Adapting Fixed-End-Point Configurational-Bias Monte Carlo Method for the Regrowth of Interior Segments of Chain Molecules with Strong Intramolecular Interactions. 2000 , 33, 7207-7218		104
1280	On the role of the definition of potential models in Gibbs ensemble phase equilibria simulations of the H ₂ S-pentane mixture. <i>Molecular Physics</i> , 2000 , 98, 1895-1905	1.7	24
1279	Thermodynamic and transport properties of nitrogen and butane mixtures. <i>Molecular Physics</i> , 2000 , 98, 43-55	1.7	28
1278	A Comprehensive Liquid Simulation Study of Neat Formic Acid. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 8287-8294	3.4	30
1277	A Novel Monte Carlo Algorithm for Simulating Strongly Associating Fluids: Applications to Water, Hydrogen Fluoride, and Acetic Acid. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 8725-8734	3.4	150

1276	The Zeno ($Z = 1$) Behavior of Equations of State: An Interpretation across Scales from Macroscopic to Molecular. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 9513-9525	3.4	51
1275	Derivation of an Optimized Potential Model for Phase Equilibria (OPPE) for Sulfides and Thiols. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 4745-4753	3.4	60
1274	Partitioning of Alkane and Alcohol Solutes between Water and (Dry or Wet) 1-Octanol. 2000 , 122, 6464-6467		53
1273	Development of Polarizable Water Force Fields for Phase Equilibrium Calculations. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 2391-2401	3.4	200
1272	Monte Carlo simulations of neon and argon using ab initio potentials. <i>Molecular Physics</i> , 2000 , 98, 1603-1616	3.4	45
1271	Molecular Structure and Phase Diagram of the Binary Mixture of n-Heptane and Supercritical Ethane: A Gibbs Ensemble Monte Carlo Study. <i>Journal of Physical Chemistry B</i> , 2000 , 104, 2415-2423	3.4	19
1270	Surface tension of the three-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2000 , 112, 6411-6415	3.9	133
1269	Simulation of vapour-liquid equilibria for branched alkanes. <i>Molecular Physics</i> , 2000 , 98, 231-238	1.7	66
1268	Hyperparallel tempering Monte Carlo simulation of polymeric systems. <i>Journal of Chemical Physics</i> , 2000 , 113, 1276-1282	3.9	96
1267	The effect of force-field parameters on properties of liquids: Parametrization of a simple three-site model for methanol. <i>Journal of Chemical Physics</i> , 2000 , 112, 10450-10459	3.9	120
1266	Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary, and Tertiary Alcohols. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 3093-3104	3.4	632
1265	Vapour-Liquid Phase Equilibria of n-alkanes by Direct Monte Carlo Simulations. 2001 , 27, 99-114		37
1264	Inadequacy of the Lorentz-Berthelot combining rules for accurate predictions of equilibrium properties by molecular simulation. <i>Molecular Physics</i> , 2001 , 99, 619-625	1.7	236
1263	Coexistence and criticality of fluids with long-range potentials. <i>Journal of Chemical Physics</i> , 2001 , 114, 399	3.9	45
1262	Some chemical engineering applications of quantum chemical calculations. 2001 , 28, 313-351		2
1261	Density functional theories and molecular simulations of adsorption and phase transitions in nanopores. 2001 , 64, 011602		249
1260	Properties of 2,2,2-trifluoroethanol and water mixtures. <i>Journal of Chemical Physics</i> , 2001 , 114, 426	3.9	83
1259	Critical Properties of Lennard-Jones Fluids in Narrow Slit-Shaped Pores. 2001 , 17, 4451-4458		77

1258	Modelling Gas Adsorption in Slit-Pores Using Monte Carlo Simulation. 2001 , 27, 295-321		31
1257	Improving the Efficiency of the Aggregation-Volume-Bias Monte Carlo Algorithm. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 11275-11282	3-4	109
1256	Simulation of Ternary Mixtures of Ethylene, 1-Hexene, and Polyethylene. 2001 , 34, 7841-7848		36
1255	Computer simulation of fluid phase transitions. 2001 , 69, 1147-1155		86
1254	Liquid-Liquid-Vapor, Liquid-Liquid, and Liquid-Vapor Phase Transitions in Aqueous n-Hexane Mixtures from Isochoric Heat Capacity Measurements. 2001 , 46, 1556-1567		56
1253	Chemical equilibria in slitlike pores. <i>Journal of Chemical Physics</i> , 2001 , 114, 5397-5403	3-9	26
1252	Effect of pressure, membrane thickness, and placement of control volumes on the flux of methane through thin silicalite membranes: A dual control volume grand canonical molecular dynamics study. <i>Journal of Chemical Physics</i> , 2001 , 114, 7174-7181	3-9	67
1251	Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. 2001 , 42, 83-129		74
1250	Method for liquid-vapor coexistence curves by test-particle insertions in the canonical ensemble. 2001 , 293-295, 715-718		2
1249	Characterization of Porous Materials by Gas Adsorption at Ambient Temperatures and High Pressure. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 1403-1411	3-4	60
1248	Phase coexistence and critical point determination in polydisperse fluids. <i>Molecular Physics</i> , 2001 , 99, 167-173	1-7	14
1247	Direct calculation of bubble points for alkane mixtures by molecular simulation. <i>Molecular Physics</i> , 2001 , 99, 1423-1434	1-7	18
1246	New forcefield parameters for branched hydrocarbons. <i>Journal of Chemical Physics</i> , 2001 , 115, 10837-10844	3-9	59
1245	Pair approximation for polarization interaction: efficient method for Monte Carlo simulations of polarizable fluids. <i>Molecular Physics</i> , 2001 , 99, 349-354	1-7	19
1244	Examination of Chain Length Effects on the Solubility of Alkanes in Near-Critical and Supercritical Aqueous Solutions. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 841-847	3-4	23
1243	Direct Gibbs Ensemble Monte Carlo Simulations for Solid-Vapor Phase Equilibria: Applications to Lennard-Jonesium and Carbon Dioxide. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 9840-9848	3-4	87
1242	Simulation Studies of Retention in Isotropic or Oriented Liquid n-Octadecane. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 10961-10966	3-4	7
1241	Dynamics of Exchange at Gas-Zeolite Interfaces I: Pure Component n-Butane and Isobutane. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 5700-5712	3-4	26

1240	4. Molecular Simulations of Liquid and Supercritical Water: Thermodynamics, Structure, and Hydrogen Bonding. 2001 , 83-130		13
1239	A new simulation method for the determination of phase equilibria in mixtures in the grand canonical ensemble. <i>Molecular Physics</i> , 2001 , 99, 2011-2022	1.7	15
1238	Hyperparallel tempering Monte Carlo and its applications. 2001 , 28, 1-20		1
1237	Expansion Type of Model Fluids. 2001 , 70, 1006-1009		14
1236	Molecular simulation study on the colloidal suspension within dilute fibrous media: The effect of particle concentration on partitioning. 2001 , 18, 816-823		3
1235	Fluid-fluid phase equilibria in disordered porous media. Nonadditive hard sphere mixture. 2001 , 280, 146-152		13
1234	Molecular dynamics investigations on Lennard-Jones systems near the gas-liquid critical point. <i>Fluid Phase Equilibria</i> , 2001 , 178, 97-118	2.5	6
1233	Phase behavior of amphiphile-solvent systems from lattice Monte Carlo simulations. <i>Fluid Phase Equilibria</i> , 2001 , 179, 193-206	2.5	4
1232	Comprehensive study of the vapour-liquid equilibria of the pure two-centre Lennard-Jones plus pointquadrupole fluid. <i>Fluid Phase Equilibria</i> , 2001 , 179, 339-362	2.5	67
1231	Coexistence properties of higher n-alkanes modelled as Kihara fluids: Gibbs ensemble simulations. <i>Fluid Phase Equilibria</i> , 2001 , 181, 83-94	2.5	3
1230	Monte Carlo simulation of phase equilibria of aqueous systems. <i>Fluid Phase Equilibria</i> , 2001 , 183-184, 259-269	2.5	17
1229	Chain length effects on aqueous alkane solubility near the solvent's critical point. <i>Fluid Phase Equilibria</i> , 2001 , 183-184, 289-294	2.5	3
1228	Monte Carlo calculations for the phase equilibria of alkanes, alcohols, water, and their mixtures. <i>Fluid Phase Equilibria</i> , 2001 , 183-184, 301-309	2.5	40
1227	Accurate vapour-liquid equilibrium calculations for complex systems using the reaction Gibbs ensemble Monte Carlo simulation method. <i>Fluid Phase Equilibria</i> , 2001 , 181, 127-146	2.5	67
1226	Molecular dynamics simulation for Henry's constant of oxygen in benzene. <i>Fluid Phase Equilibria</i> , 2001 , 187-188, 29-37	2.5	14
1225	Histogram reweighting and finite-size scaling study of the Lennard-Jones fluids. <i>Fluid Phase Equilibria</i> , 2001 , 187-188, 171-191	2.5	66
1224	On the mean spherical approximation for the Lennard-Jones fluid. <i>Fluid Phase Equilibria</i> , 2001 , 190, 149-158		26
1223	Water in porous carbons. 2001 , 187-188, 539-568		314

1222	Phase behavior of C60 by computer simulation using ab-initio interaction potential. 2001 , 84, 375-387		4
1221	Molecular simulation of complete phase diagrams for binary mixtures. 2001 , 47, 1664-1675		35
1220	Vapor-liquid equilibria of mixtures containing alkanes, carbon dioxide, and nitrogen. 2001 , 47, 1676-1682		1229
1219	The starting state in simulations of the fluid-solid coexistence by Gibbs-Duhem integration. 2001 , 141, 403-411		7
1218	Reliable Determination of the Liquid-Vapor Critical Point by the NVT-Plus Test Particle Method. 2001 , 70, 1990-1994		44
1217	The liquid-vapour interface of pure fluids and mixtures: application of computer simulation and density functional theory. <i>Journal of Physics Condensed Matter</i> , 2001 , 13, 4739-4768	1.8	44
1216	Phase behavior of a simple model for membrane proteins. <i>Journal of Chemical Physics</i> , 2001 , 114, 2477-2483	3.9	17
1215	A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in polymer melts: Solubility of long alkanes in linear polyethylene. <i>Journal of Chemical Physics</i> , 2001 , 115, 2860-2875	3.9	29
1214	Approximate integral equation theory for classical fluids. <i>Journal of Chemical Physics</i> , 2001 , 114, 9496-9505	3.9	41
1213	Phase behavior of monomeric mixtures and polymer solutions with soft interaction potentials. <i>Journal of Chemical Physics</i> , 2001 , 114, 7644-7654	3.9	102
1212	The isotropic-nematic transition in hard Gaussian overlap fluids. <i>Journal of Chemical Physics</i> , 2001 , 115, 9072-9083	3.9	32
1211	Crystalline ground states of an entropically stabilized quasicrystal model. 2001 , 64,		12
1210	Simple model of liquid-liquid phase transitions. 2001 , 64,		13
1209	A new united atom force field for olefins. <i>Journal of Chemical Physics</i> , 2001 , 114, 3612-3616	3.9	70
1208	Simulation of bulk, confined, and polydisperse systems. I. A unified methodological framework. <i>Journal of Chemical Physics</i> , 2001 , 115, 5642-5652	3.9	26
1207	Computing phase equilibria by parallel excluded volume tempering. <i>Journal of Chemical Physics</i> , 2001 , 115, 8731-8741	3.9	8
1206	Influence of solute-solvent interactions on the local solvent density augmentation in supercritical fluids: An integral equation study. <i>Journal of Chemical Physics</i> , 2001 , 115, 6115-6129	3.9	11
1205	Aggregation-volume-bias Monte Carlo simulations of vapor-liquid nucleation barriers for Lennard-Jonesium. <i>Journal of Chemical Physics</i> , 2001 , 115, 10903-10913	3.9	107

- 1204 Weighted density-functional theory for simple fluids: prewetting of a Lennard-Jones fluid. **2002**, 65, 011102 34
- 1203 Comparison of polarizable and nonpolarizable models of hydrogen fluoride in liquid and supercritical states: A Monte Carlo simulation study. *Journal of Chemical Physics*, **2001**, 115, 9883-9894 3.9 10
- 1202 Phase separation of binary homopolymer and ternary homopolymer-dopolymer mixtures through Gibbs ensemble simulations. *Journal of Chemical Physics*, **2001**, 114, 8174-8180 3.9 6
- 1201 Role of anisotropic interactions in protein crystallization. **2002**, 66, 011909 25
- 1200 New criteria for cluster identification in continuum systems. *Journal of Chemical Physics*, **2002**, 116, 10973-1108 27
- 1199 Pair approximation for polarization interaction and adiabatic nuclear and electronic sampling method for fluids with dipole polarizability. *Molecular Physics*, **2002**, 100, 2703-2717 1.7 13
- 1198 Grand Equilibrium: vapour-liquid equilibria by a new molecular simulation method. *Molecular Physics*, **2002**, 100, 3375-3383 1.7 113
- 1197 Prediction of the phase behavior of acetonitrile and methanol with ab initio pair potentials. I. Pure components. *Journal of Chemical Physics*, **2002**, 116, 7627-7636 3.9 27
- 1196 Development of a force field for molecular simulation of the phase equilibria of perfluoromethylpropyl ether. *Molecular Physics*, **2002**, 100, 265-272 1.7 16
- 1195 Self-referential method for calculation of the free energy of crystals by Monte Carlo simulation. **2002**, 65, 036709 8
- 1194 Computation of a chemical potential using a residence weight algorithm. **2002**, 66, 046705 23
- 1193 Monte Carlo simulation of vapor-liquid binodal of water. *Journal of Chemical Physics*, **2002**, 117, 9518-9519 3.9 7
- 1192 Adsorption of selenium wires in silicalite-1 zeolite: a first order transition in a microporous system. **2002**, 89, 016101 21
- 1191 On the application of virtual Gibbs ensembles to the direct simulation of fluid-fluid and solid-fluid phase coexistence. *Journal of Chemical Physics*, **2002**, 116, 7957-7966 3.9 9
- 1190 Gibbs ensemble Monte Carlo simulations of coexistence properties of a polarizable potential model of water. *Journal of Chemical Physics*, **2002**, 117, 3522-3523 3.9 21
- 1189 Monte Carlo simulation of branched alkanes and long chain n-alkanes with anisotropic united atoms intermolecular potential. **2002**, 28, 317-336 75
- 1188 Molecular Modeling. **2002**, 1188, 011102 25
- 1187 A 2-Site Model for Simulating Supercritical Fluoroform. *Journal of Physical Chemistry B*, **2002**, 106, 8783-8789 3.9 18

- 1186 A grand canonical Monte Carlo simulation study of water adsorption in a Vycor-like disordered mesoporous material at 300K.. **2002**, 371-378
- 1185 Bibliography. **2002**, 589-617
- 1184 Vapour-liquid equilibrium of the square-well fluid of variable range via a hybrid simulation approach. *Molecular Physics*, **2002**, 100, 2531-2546 1.7 92
- 1183 Influence of Analyte Overloading on Retention in Gas-liquid Chromatography: A Molecular Simulation View. **2002**, 74, 37-44 13
- 1182 Molecular Simulation of the High-Pressure Phase Equilibrium of the System Carbon Dioxide-Methanol-Water. *Journal of Physical Chemistry B*, **2002**, 106, 7547-7553 3-4 16
- 1181 Monte Carlo Simulation of the Phase Diagram of C60 Using Two Interaction Potentials. Enthalpies of Sublimation. *Journal of Physical Chemistry B*, **2002**, 106, 10227-10232 3-4 17
- 1180 Prediction of Equilibrium Properties of Cyclic Alkanes by Monte Carlo Simulation New Anisotropic United Atoms Intermolecular Potential New Transfer Bias Method. *Journal of Physical Chemistry B*, **2002**, 106, 5483-5491 3-4 81
- 1179 Vapor-liquid interfacial properties of mutually saturated water/1-butanol solutions. **2002**, 124, 12232-7 70
- 1178 Phase Coexistence Curves for Off-Lattice Polymer-Solvent Mixtures: Gibbs-Ensemble Simulations. **2002**, 35, 2827-2834 18
- 1177 Molecular simulation of concurrent gas-liquid interfacial adsorption and partitioning in gas-liquid chromatography. **2002**, 74, 3518-24 33
- 1176 Influence of polymer-excluded volume on the phase-behavior of colloid-polymer mixtures. **2002**, 89, 128302 174
- 1175 Monte Carlo Methods for Bridging the Timescale Gap. **2002**, 231-266 4
- 1174 Simulating vapor-liquid nucleation of n-alkanes. *Journal of Chemical Physics*, **2002**, 116, 4317-4329 3-9 57
- 1173 The melting lines of model systems calculated from coexistence simulations. *Journal of Chemical Physics*, **2002**, 116, 9352-9358 3-9 232
- 1172 Direct Monte Carlo simulations of the equilibrium properties of n-pentane liquid-vapor interface. *Journal of Chemical Physics*, **2002**, 116, 8106-8117 3-9 73
- 1171 Molecular simulation of phase coexistence in adsorption in porous solids. *Molecular Physics*, **2002**, 100, 3803-3815 1.7 47
- 1170 An examination of the five-site potential (TIP5P) for water. *Journal of Chemical Physics*, **2002**, 117, 8892-8897 3-9 85
- 1169 New formula for the bulk viscosity constructed from the interatomic potential and the pair distribution function. *Journal of Chemical Physics*, **2002**, 116, 7400-7410 3-9 25

1168	Monte Carlo simulations of nitrogen using an ab initio potential. <i>Molecular Physics</i> , 2002 , 100, 2571-2585.	1.7	30
1167	Phase transitions of one-component fluids adsorbed in random porous media: Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2002 , 116, 8948-8958	3.9	36
1166	Solid-liquid coexistence of the Lennard-Jones system from absolute free energy calculations. <i>Journal of Chemical Physics</i> , 2002 , 116, 7145-7150	3.9	70
1165	Prediction of the vapor-liquid phase equilibrium of hydrogen sulfide and the binary system water-hydrogen sulfide by molecular simulation. 2002 , 4, 4449-4457		20
1164	Molecular Dynamics Study of the Structure and Thermophysical Properties of Model sl Clathrate Hydrates. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 442-451	3.4	94
1163	Solvation forces and liquid-solid phase equilibria for water confined between hydrophobic surfaces. <i>Journal of Chemical Physics</i> , 2002 , 116, 10882-10889	3.9	32
1162	Monte Carlo and cell model calculations for the solid-liquid phase behaviour of the triangle-well model. <i>Molecular Physics</i> , 2002 , 100, 1543-1550	1.7	12
1161	The extrapolation of phase equilibrium curves of mixtures in the isobaric-isothermal Gibbs ensemble. <i>Molecular Physics</i> , 2002 , 100, 3429-3441	1.7	8
1160	Phase behavior of mixtures of colloidal platelets and nonadsorbing polymers. <i>Journal of Chemical Physics</i> , 2002 , 117, 9947-9958	3.9	63
1159	The extrapolation of the vapour-liquid equilibrium curves of pure fluids in the isothermal Gibbs ensemble. <i>Molecular Physics</i> , 2002 , 100, 1989-2000	1.7	6
1158	Phase equilibria of the system methane-ethane from temperature scaling Gibbs Ensemble Monte Carlo simulation. 2002 , 66, 3431-3439		13
1157	Computer simulation of liquid semiconductors. 2002 , 312-314, 341-348		5
1156	Molecular and Mesoscale Simulation Methods for Polymer Materials. 2002 , 32, 401-436		165
1155	Molecular simulations in chemical engineering: Present and future. 2002 , 48, 2716-2721		43
1154	A reappraisal of what we have learnt during three decades of computer simulations on water. 2002 , 101, 219-260		752
1153	The use of quantum chemistry to predict phase behavior for environmental and process engineering. <i>Fluid Phase Equilibria</i> , 2002 , 194-197, 61-75	2.5	15
1152	Thermodynamic properties of freely-jointed hard-sphere multi-Yukawa chain fluids: theory and simulation. <i>Fluid Phase Equilibria</i> , 2002 , 194-197, 185-196	2.5	10
1151	Web-based technologies for teaching and using molecular simulation. <i>Fluid Phase Equilibria</i> , 2002 , 194-197, 327-335	2.5	15

1150	Ab initio pair potentials and phase equilibria predictions of halogenated compounds. <i>Fluid Phase Equilibria</i> , 2002 , 199, 5-13	2.5	13
1149	Pressure-enthalpy driven molecular dynamics for thermodynamic property calculation. <i>Fluid Phase Equilibria</i> , 2002 , 200, 75-92	2.5	15
1148	Pressure-enthalpy driven molecular dynamics for thermodynamic property calculation II: applications. <i>Fluid Phase Equilibria</i> , 2002 , 200, 93-110	2.5	23
1147	Vapor-liquid phase equilibria of triacontane isomers: Deviations from the principle of corresponding states. <i>Fluid Phase Equilibria</i> , 2002 , 202, 307-324	2.5	27
1146	Location of phase equilibria by temperature-quench molecular dynamics simulations. <i>Fluid Phase Equilibria</i> , 2002 , 203, 1-14	2.5	37
1145	A polarizable force field for water using an artificial neural network. 2002 , 641, 77-91		43
1144	Phase behavior and physico-chemical properties of aqueous electrolyte solutions near the critical point via molecular dynamics simulation with gravity perturbation. <i>Fluid Phase Equilibria</i> , 2002 , 194-197, 271-280	2.5	5
1143	Phase diagrams of hexadecane-CO ₂ mixtures from histogram-reweighting Monte Carlo. 2002 , 147, 378-381		24
1142	A new simulation approach to the freezing transition. 2002 , 146, 99-106		14
1141	Temperature effects on the retention of n-alkanes and arenes in helium-squalane gas-liquid chromatography. Experiment and molecular simulation. 2002 , 954, 181-90		54
1140	Chemical potential of quadrupolar two-centre Lennard-Jones fluids by gradual insertion. 2002 , 356, 431-436		46
1139	Confinement effect on thermodynamic and structural properties of water in hydrophilic mesoporous silica. 2003 , 12 Suppl 1, S67-70		13
1138	Vapor-liquid equilibria of mixtures containing nitrogen, oxygen, carbon dioxide, and ethane. 2003 , 49, 2187-2198		71
1137	Parallel tempering-cavity-bias algorithm in the Gibbs ensemble. 2003 , 368, 452-457		8
1136	Parallel Monte Carlo simulations by asynchronous domain decomposition. 2003 , 155, 31-41		11
1135	Development of an all-atoms force field from ab initio calculations for alternative refrigerants. <i>Fluid Phase Equilibria</i> , 2003 , 210, 105-116	2.5	25
1134	Continuum percolation of simple fluids: energetic connectivity criteria. 2003 , 321, 398-410		5
1133	New expression of the bulk viscosity. 2003 , 321, 207-219		22

1132	Vapour-liquid coexistence properties and critical points of two branched alkanes series. <i>Fluid Phase Equilibria</i> , 2003 , 208, 123-139	2.5	9
1131	Vapor-liquid equilibria of the binary mixtures nitrogen + methane, nitrogen + ethane and nitrogen + carbon dioxide, and the ternary mixture nitrogen + methane + ethane from Gibbs-ensemble molecular simulation. <i>Fluid Phase Equilibria</i> , 2003 , 208, 155-169	2.5	18
1130	A simulation study of the quantum hard-sphere Yukawa fluid. <i>Journal of Chemical Physics</i> , 2003 , 119, 10256-10267	3.9	16
1129	Evaluating surface tension using grand-canonical transition-matrix Monte Carlo simulation and finite-size scaling. 2003 , 67, 012102		147
1128	Surface tension of a square well fluid. <i>Journal of Chemical Physics</i> , 2003 , 118, 5635-5639	3.9	49
1127	The phase behavior of a binary mixture of rodlike and disclike mesogens: Monte Carlo simulation, theory, and experiment. <i>Journal of Chemical Physics</i> , 2003 , 119, 5216-5225	3.9	54
1126	Phase Diagrams and Sublimation Enthalpies of Model C ₆₀ Fullerenes: A Comparative Study by Computer Simulation. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 276-281	3.4	10
1125	Isotherms for the liquid-gas phase transition in silicon from NPT Monte Carlo simulations. 2003 , 67,		17
1124	Further Validation of a Set of Quadrupolar Potential Models for Ethylene and Propylene from the Prediction of some Binary Mixture Vapor-Liquid Equilibria by Gibbs-ensemble Molecular Simulation. 2003 , 29, 549-554		14
1123	Integral Equation Prediction of Reversible Coagulation in Charged Colloidal Suspensions. 2003 , 19, 475-482		17
1122	Direct calculation of liquid-vapor phase equilibria from transition matrix Monte Carlo simulation. <i>Journal of Chemical Physics</i> , 2003 , 118, 9915-9925	3.9	245
1121	Surface tension and vapor-liquid phase coexistence of the square-well fluid. <i>Journal of Chemical Physics</i> , 2003 , 119, 3405-3412	3.9	126
1120	Molecular-dynamics study of ablation of solids under femtosecond laser pulses. 2003 , 67,		246
1119	Computational chemistry for molecular electronics. 2003 , 28, 321-341		40
1118	Fluid-solid equilibria of flexible and linear rigid tangent chains from Wertheim's thermodynamic perturbation theory. <i>Journal of Chemical Physics</i> , 2003 , 119, 10958-10971	3.9	14
1117	Molecular Simulation of Vapor-Liquid Phase Equilibria of Hydrogen Sulfide and Its Mixtures with Alkanes. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 9498-9504	3.4	62
1116	Temperature Dependence of Transfer Properties: Importance of Heat Capacity Effects. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 10623-10627	3.4	18
1115	Simulation of the coexistence of a shearing liquid and a strained crystal. <i>Journal of Chemical Physics</i> , 2003 , 118, 4115-4126	3.9	31

1114	Isotopic effect on phase equilibria of atomic fluids and their mixtures: A direct comparison between molecular simulation and experiment. <i>Journal of Chemical Physics</i> , 2003 , 119, 4458-4467	3.9	13
1113	Fluid-fluid coexistence in colloidal systems with short-ranged strongly directional attraction. <i>Journal of Chemical Physics</i> , 2003 , 118, 9882-9889	3.9	401
1112	Grand canonical Monte Carlo simulation study of water structure on hydrophilic mesoporous and plane silica substrates. <i>Journal of Chemical Physics</i> , 2003 , 119, 9226-9232	3.9	57
1111	A density-functional theory for bulk and inhomogeneous Lennard-Jones fluids from the energy route. <i>Journal of Chemical Physics</i> , 2003 , 119, 7388-7397	3.9	55
1110	Hydrogen fluoride phase behavior and molecular structure: Ab initio derived potential models. <i>Journal of Chemical Physics</i> , 2003 , 119, 6092-6099	3.9	17
1109	An optimized potential for phase equilibria calculation for ketone and aldehyde molecular fluids. 2003 , 5, 4175-4179		16
1108	Grand canonical Monte Carlo simulations of phase equilibria of pure silicon tetrachloride and its binary mixture with carbon dioxide. <i>Molecular Physics</i> , 2003 , 101, 3213-3221	1.7	6
1107	Nitrogen adsorption on carbon nanotube bundles: Role of the external surface. 2003 , 68,		59
1106	The phase diagram of the two center Lennard-Jones model as obtained from computer simulation and Wertheim's thermodynamic perturbation theory. <i>Journal of Chemical Physics</i> , 2003 , 118, 10696-10706	3.9	30
1105	A simulation study of lyotropic isotropic-nematic phase transitions in polydisperse chain systems. <i>Journal of Chemical Physics</i> , 2003 , 118, 10262-10275	3.9	13
1104	Gibbs ensemble simulation of symmetric mixtures composed by the homopolymers AA, BB and their common block copolymer AB. <i>Journal of Chemical Physics</i> , 2003 , 118, 425-433	3.9	11
1103	Boolean Scheme for Programming Trial Moves That Involve Molecule Insertion and Removal in Monte Carlo Simulation. 2003 , 29, 23-28		1
1102	Simulation of phase equilibria and interfacial properties of binary mixtures on the liquid-vapour interface using lattice sums. <i>Molecular Physics</i> , 2003 , 101, 743-751	1.7	29
1101	Critical properties of molecular fluids from the virial series. <i>Journal of Chemical Physics</i> , 2003 , 119, 11367-11373	3.9	17
1100	Scaling behavior for the pressure and energy of shearing fluids. 2003 , 67, 061201		20
1099	Monte Carlo simulations for the phase behavior of symmetric nonadditive hard sphere mixtures. <i>Journal of Chemical Physics</i> , 2003 , 118, 7907-7911	3.9	28
1098	Prediction of thermodynamic properties of krypton by Monte Carlo simulation using ab initio interaction potentials. <i>Journal of Chemical Physics</i> , 2003 , 119, 947-952	3.9	40
1097	Water adsorption on hydrophilic mesoporous and plane silica substrates: A grand canonical Monte Carlo simulation study. <i>Journal of Chemical Physics</i> , 2003 , 118, 5613-5622	3.9	85

1096	Ab initio pair potential and phase equilibria predictions for hydrogen chloride. <i>Journal of Chemical Physics</i> , 2003 , 118, 4086-4093	3.9	20
1095	Equilibrium and nonequilibrium molecular dynamics methods for determining solid-liquid phase coexistence at equilibrium. <i>Journal of Chemical Physics</i> , 2003 , 119, 11017-11023	3.9	21
1094	Monte Carlo simulations using sampling from an approximate potential. <i>Journal of Chemical Physics</i> , 2003 , 118, 7747-7750	3.9	72
1093	Phase behavior of lattice associating binary mixtures: a Monte Carlo study. 2003 , 67, 031202		1
1092	Direct molecular-level Monte Carlo simulation of Joule-Thomson processes. <i>Molecular Physics</i> , 2003 , 101, 2875-2884	1.7	20
1091	Binary mixtures of magnetic fluids. 2003 , 67, 021507		11
1090	Equation of state of supercooled water from the sedimentation profile. 2003 , 67, 010202		15
1089	Determination of liquid-solid transition using histogram reweighting method and expanded ensemble simulations. <i>Journal of Chemical Physics</i> , 2003 , 118, 8390-8395	3.9	42
1088	New optimization method for intermolecular potentials: Optimization of a new anisotropic united atoms potential for olefins: Prediction of equilibrium properties. <i>Journal of Chemical Physics</i> , 2003 , 118, 3020-3034	3.9	137
1087	Application of molecular simulation in the gibbs ensemble to predict liquid-vapor equilibrium curve of acetonitrile. 2003 , 14, 653-658		1
1086	On the development of a general force field for the molecular simulation of perfluoroethers. <i>Molecular Physics</i> , 2003 , 101, 2157-2169	1.7	24
1085	Phase coexistence in a DLVO model of globular protein solutions. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, 375-384	1.8	38
1084	Capillary condensation of colloid-polymer mixtures confined between parallel plates. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, S3411-S3420	1.8	37
1083	Cloud and solubility temperatures versus ionic strength in model lysozyme solutions. <i>Journal of Physics Condensed Matter</i> , 2003 , 15, S3485-S3489	1.8	5
1082	A Thermodynamic-scaling Study of Gibbs-ensemble Monte Carlo. 2003 , 29, 627-642		6
1081	Towards the atomistic description of equilibrium-based separation processes. 1. Isothermal stirred-tank adsorber. 2003 , 14, 791-796		
1080	From Organic Geochemistry to Statistical Thermodynamics: the Development of Simulation Methods for the Petroleum Industry. 2003 , 58, 271-297		6
1079	Interatomic Lennard-Jones potentials of linear and branched alkanes calibrated by Gibbs ensemble simulations for vapor-liquid equilibria. <i>Journal of Chemical Physics</i> , 2004 , 121, 7474-83	3.9	34

1078	Anomalous mixing behavior of polyisobutylene/polypropylene blends: molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2004 , 120, 8883-6	3.9	34
1077	Binary phase behavior and aggregation of dilute methanol in supercritical carbon dioxide: a Monte Carlo simulation study. <i>Journal of Chemical Physics</i> , 2004 , 121, 1525-34	3.9	60
1076	Phase behavior of n-alkanes in supercritical solution: a Monte Carlo study. <i>Journal of Chemical Physics</i> , 2004 , 121, 2169-79	3.9	88
1075	Simulation of the effects of chain architecture on the sorption of ethylene in polyethylene. <i>Journal of Chemical Physics</i> , 2004 , 120, 11304-15	3.9	41
1074	A finite-size scaling study of a model of globular proteins. <i>Journal of Chemical Physics</i> , 2004 , 120, 8292-83.9	3.9	7
1073	Capillary evaporation in colloid-polymer mixtures selectively confined to a planar slit. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S4159-S4168	1.8	23
1072	Theory and simulation of short-range models of globular protein solutions. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S4923-S4936	1.8	36
1071	Molecular Simulation of Phase Equilibria for Industrial Applications. 2004 , 279-307		1
1070	Application of Gibbs Ensemble and NPT Monte Carlo Simulation to the Development of Improved Processes for H ₂ S-rich Gases. 2004 , 30, 631-648		33
1069	Gibbs Ensemble Monte Carlo Simulation of LJ Fluid in Cylindrical Pore with Energetically Heterogeneous Surface. 2004 , 30, 353-359		3
1068	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 2. Alkylbenzenes and Styrene. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 14115-14123	3.4	34
1067	Optimized Intermolecular Potential for Aromatic Hydrocarbons Based on Anisotropic United Atoms. 1. Benzene. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 14109-14114	3.4	48
1066	Molecular simulation of vapor-liquid equilibria of toxic gases. <i>Fluid Phase Equilibria</i> , 2004 , 220, 1-6	2.5	7
1065	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. <i>Fluid Phase Equilibria</i> , 2004 , 224, 73-81	2.5	17
1064	Effect of pressure on the complete phase behavior of binary mixtures. 2004 , 50, 215-225		13
1063	Thermodynamics of fluid-phase equilibria for standard chemical engineering operations. 2004 , 50, 739-761		155
1062	Monte Carlo simulations of vapor-liquid equilibria of neon using an accurate ab initio pair potential. <i>Fluid Phase Equilibria</i> , 2004 , 218, 285-289	2.5	22
1061	Measurement and prediction of vapour pressures of 2,6,10,14-tetramethylpentadecane (pristane). <i>Fluid Phase Equilibria</i> , 2004 , 225, 49-57	2.5	1

1060	Molecular simulation of the solubility of carbon dioxide in aqueous solutions of sodium chloride. <i>Fluid Phase Equilibria</i> , 2004 , 226, 237-250	2.5	23
1059	Grand canonical auxiliary field Monte Carlo: a new technique for simulating open systems at high density. 2004 , 157, 201-206		12
1058	The Extrapolation of Vapour-Liquid Equilibrium Curves of Pure Fluids in Alternative Gibbs Ensemble Monte Carlo Implementations. 2004 , 30, 549-558		
1057	Molecular simulation of binary vapour-liquid equilibria with components differing largely in volatility. <i>Molecular Physics</i> , 2004 , 102, 301-317	1.7	5
1056	Polymorphism in simple liquids: a Gibbs ensemble Monte Carlo study. <i>Journal of Chemical Physics</i> , 2004 , 120, 8671-5	3.9	8
1055	Computer simulation study of the global phase behavior of linear rigid Lennard-Jones chain molecules: comparison with flexible models. <i>Journal of Chemical Physics</i> , 2004 , 120, 3957-68	3.9	25
1054	Liquid crystalline behavior of a semifluorinated oligomer. <i>Journal of Chemical Physics</i> , 2004 , 121, 11463-73	3.9	21
1053	Monte Carlo Simulations of Disjoining-Pressure Isotherms for Lennard-Jones Surfactant-Stabilized Free Thin Films. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 13412-13418	3.4	8
1052	Gibbs Ensemble Simulations of Vapor/Liquid Equilibrium Using the Flexible RWK2 Water Potential. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 20303-20309	3.4	16
1051	Monte Carlo Simulation of Formic Acid Dimerization in a Carbon Dioxide Solvent. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 11716-11721	3.4	9
1050	Prediction of the thermophysical properties of pure neon, pure argon, and the binary mixtures neon-argon and argon-krypton by Monte Carlo simulation using ab initio potentials. <i>Journal of Chemical Physics</i> , 2004 , 121, 6423-34	3.9	72
1049	HM-IE: Quantum Chemical Hybrid Methods for Calculating Interaction Energies. 2004 , 108, 107-112		43
1048	Microscopic Determination of the Phase Diagrams of Lysozyme and β -Crystallin Solutions. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 7538-7541	3.4	35
1047	Simulation of Vapor-Liquid Phase Equilibria of Primary Alcohols and Alcohol-Alkane Mixtures. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 10071-10076	3.4	34
1046	Simulation studies on the effects of mobile-phase modification on partitioning in liquid chromatography. 2004 , 76, 2886-92		16
1045	Understanding the Limitations of the Virial in the Simulation of Nanosystems: A Puzzle That Stimulated the Search for Understanding. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 6555-6563	3.4	9
1044	Water in nanopores. I. Coexistence curves from Gibbs ensemble Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2004 , 120, 1958-72	3.9	109
1043	Transferable Potentials for Phase Equilibria. 6. United-Atom Description for Ethers, Glycols, Ketones, and Aldehydes. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 17596-17605	3.4	355

1042	Constrained fluid lambda-integration: constructing a reversible thermodynamic path between the solid and liquid state. <i>Journal of Chemical Physics</i> , 2004 , 120, 2122-6	3.9	104
1041	Oppositely charged colloidal binary mixtures: a colloidal analog of the restricted primitive model. <i>Journal of Chemical Physics</i> , 2004 , 121, 2428-35	3.9	26
1040	The role of fluctuations in both density functional and field theory of nanosystems. <i>Journal of Chemical Physics</i> , 2004 , 120, 2558-64	3.9	33
1039	Grand canonical Monte Carlo simulation of a model colloid-polymer mixture: coexistence line, critical behavior, and interfacial tension. <i>Journal of Chemical Physics</i> , 2004 , 121, 3253-8	3.9	100
1038	Stationary dynamics approach to analytical approximations for polymer coexistence curves. 2004 , 69, 021808		1
1037	Simulating Fluid-Solid Equilibrium with the Gibbs Ensemble. 2004 , 30, 23-28		15
1036	Calculation of free energy through successive umbrella sampling. <i>Journal of Chemical Physics</i> , 2004 , 120, 10925-30	3.9	238
1035	An Improved Force Field for the Prediction of the Vapor-Liquid Equilibria for Carboxylic Acids. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 14130-14136	3.4	69
1034	Liquid-Gas Phase Transitions Studied by Multibaric-Multithermal Monte Carlo Simulations. 2004 , 73, 3304-3311		28
1033	Molecular Simulation of Adsorption Processes. 1. Isothermal Stirred-tank Adsorber. 2004 , 30, 387-396		5
1032	Adsorption of Lennard-Jones Fluids in Carbon Slit Pores of a Finite Length. A Computer Simulation Study. 2005 , 23, 1-18		25
1031	Two-dimensional model for mixtures of enantiomers, bent hard needles: a Monte Carlo simulation. 2005 , 345, 130-142		19
1030	Solubility of oxygen in the ionic liquid [bmim][PF ₆]: Experimental and molecular simulation results. 2005 , 37, 595-602		82
1029	Monte Carlo simulation for chemical reaction equilibrium of ammonia synthesis in MCM-41 pores and pillared clays. <i>Fluid Phase Equilibria</i> , 2005 , 231, 138-149	2.5	17
1028	Effect of quadrupole moment on the phase behavior of binary mixtures containing ethene. <i>Fluid Phase Equilibria</i> , 2005 , 234, 144-150	2.5	28
1027	Effects of potential models in the vapor-liquid equilibria and adsorption of simple gases on graphitized thermal carbon black. <i>Fluid Phase Equilibria</i> , 2005 , 236, 169-177	2.5	55
1026	Simulation of 1-alkene and n-alkane binary vapour-liquid equilibrium using different united-atom transferable force fields. <i>Fluid Phase Equilibria</i> , 2005 , 232, 136-148	2.5	4
1025	Monte Carlo molecular simulation predictions for the heat of vaporization of acetone and butyramide. <i>Fluid Phase Equilibria</i> , 2005 , 236, 53-57	2.5	28

1024	Molecular simulation study of the bonded-phase structure in reversed-phase liquid chromatography with neat aqueous solvent. 2005 , 1079, 127-35		50
1023	Surface critical behavior of fluids: Lennard-Jones fluid near a weakly attractive substrate. <i>European Physical Journal B</i> , 2005 , 44, 345-358	1.2	27
1022	Toward a Monte Carlo program for simulating vapor-liquid phase equilibria from first principles. 2005 , 169, 289-294		25
1021	Prediction of internal structure and properties in fluid model interfaces of binary and ternary liquid mixtures. <i>Fluid Phase Equilibria</i> , 2005 , 228-229, 293-302	2.5	10
1020	Prediction of thermodynamic properties of heavy hydrocarbons by Monte Carlo simulation. <i>Fluid Phase Equilibria</i> , 2005 , 228-229, 311-319	2.5	5
1019	Extension of the anisotropic united atoms intermolecular potential to amines, amides and alkanols: Application to the problems of the 2004 Fluid Simulation Challenge. <i>Fluid Phase Equilibria</i> , 2005 , 236, 25-41	2.5	41
1018	Fluid-phase diagrams of binary mixtures from constant pressure integral equations. <i>Journal of Chemical Physics</i> , 2005 , 122, 181104	3.9	11
1017	Simulations of vapor water clusters at vapor-liquid equilibrium. <i>Journal of Chemical Physics</i> , 2005 , 123, 24504	3.9	29
1016	Simulations of phase transitions in ionic systems. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, S3205-S3213	3.9	18
1015	From dimer to condensed phases at extreme conditions: accurate predictions of the properties of water by a Gaussian charge polarizable model. <i>Journal of Chemical Physics</i> , 2005 , 122, 244511	3.9	190
1014	Phase coexistence in heterogeneous porous media: a new extension to Gibbs ensemble Monte Carlo simulation method. <i>Journal of Chemical Physics</i> , 2005 , 122, 134710	3.9	26
1013	Histogram analysis as a method for determining the line tension of a three-phase contact region by Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2005 , 123, 184704	3.9	17
1012	Phase behavior of a three-dimensional core-softened model system. 2005 , 71, 065701		14
1011	Direct determination of phase behavior of square-well fluids. <i>Journal of Chemical Physics</i> , 2005 , 123, 174505	3.9	89
1010	Isomolar semigrand ensemble molecular dynamics: development and application to liquid-liquid equilibria. <i>Journal of Chemical Physics</i> , 2005 , 122, 54504	3.9	16
1009	Heat capacity in a model polydisperse ferrofluid with narrow particle size distribution. 2005 , 71, 031109		3
1008	Liquid-vapor and liquid-liquid phase equilibria of the Brodholt-Sampoli-Vallauri polarizable water model. <i>Journal of Chemical Physics</i> , 2005 , 122, 81101	3.9	56
1007	Phase behavior of short-range square-well model. <i>Journal of Chemical Physics</i> , 2005 , 122, 184515	3.9	80

1006	Phase behavior of Ising mixtures. 2005 , 71, 046104		6
1005	Vapor-liquid equilibria and thermophysical behavior of the SPC-HW model for heavy water. 2005 , 31, 1035-1042		
1004	Temperature-and-density-scaling Monte Carlo: methodology and the canonical thermodynamics of Lennard-Jonesium. 2005 , 31, 223-253		6
1003	Multicanonical schemes for mapping out free-energy landscapes of single-component and multicomponent systems. <i>Journal of Chemical Physics</i> , 2005 , 122, 164103	3.9	20
1002	Simulation and theory of fluid demixing and interfacial tension of mixtures of colloids and nonideal polymers. 2005 , 71, 051406		24
1001	Percolation of clusters with a residence time in the bond definition: Integral equation theory. 2005 , 71, 031202		6
1000	Cavity-bias sampling in reaction ensemble Monte Carlo simulations. <i>Molecular Physics</i> , 2005 , 103, 2647-2654	2.7	19
999	Temperature-quench Molecular Dynamics Simulations for Fluid Phase Equilibria. 2005 , 31, 33-43		25
998	Determination of fluid-phase behavior using transition-matrix Monte Carlo: binary Lennard-Jones mixtures. <i>Journal of Chemical Physics</i> , 2005 , 122, 064508	3.9	54
997	A unified methodological framework for the simulation of nonisothermal ensembles. <i>Journal of Chemical Physics</i> , 2005 , 123, 044110	3.9	15
996	Surface tension of a Lennard-Jones liquid under supersaturation. 2005 , 7, 2928-35		16
995	Temperature dependence of hydrogen bonding: an investigation of the retention of primary and secondary alcohols in gas-liquid chromatography. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 15118-25	3.4	14
994	Modelling gas mixture adsorption in active carbons. 2005 , 31, 667-681		15
993	Simulating vapor-liquid nucleation of water: A combined histogram-reweighting and aggregation-volume-bias Monte Carlo investigation for fixed-charge and polarizable models. 2005 , 109, 1137-45		57
992	Capillary condensation in a geometrically and a chemically heterogeneous pore: a molecular simulation study. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 4700-6	3.4	24
991	Trimer based polarization as a multibody molecular model. Application to hydrogen fluoride. 2005 , 127, 690-8		5
990	Thermodynamic characterization of fluids confined in heterogeneous pores by monte carlo simulations in the grand canonical and the isobaric-isothermal ensembles. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 8185-94	3.4	19
989	Does water condense in carbon pores?. 2005 , 21, 10219-25		101

988	Pressure dependence of the vapor-liquid-liquid phase behavior in ternary mixtures consisting of n-alkanes, n-perfluoroalkanes, and carbon dioxide. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 2911-9	3-4	72
987	Transferable potentials for phase equilibria. 7. Primary, secondary, and tertiary amines, nitroalkanes and nitrobenzene, nitriles, amides, pyridine, and pyrimidine. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 18974-82	3-4	188
986	Computer simulation of polymer networks: swelling by binary Lennard-Jones mixtures. <i>Journal of Chemical Physics</i> , 2005 , 123, 054902	3-9	5
985	Vapor-liquid and vapor-solid phase equilibria for united-atom benzene models near their triple points: the importance of quadrupolar interactions. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 5368-74	3-4	29
984	Optimized intermolecular potential for aromatic hydrocarbons based on anisotropic united atoms. III. Polyaromatic and naphthenoaromatic hydrocarbons. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 2970-6	3-4	46
983	Solubility of CO ₂ , CO, and H ₂ in the ionic liquid [bmim][PF ₆] from Monte Carlo simulations. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 12154-9	3-4	90
982	Transferable potentials for phase equilibria. 8. United-atom description for thiols, sulfides, disulfides, and thiophene. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 24100-7	3-4	96
981	The melting temperature of the most common models of water. <i>Journal of Chemical Physics</i> , 2005 , 122, 114507	3-9	302
980	A simulation method for the calculation of chemical potentials in small, inhomogeneous, and dense systems. <i>Journal of Chemical Physics</i> , 2005 , 122, 234108	3-9	41
979	Interfacial tension of the isotropic-nematic interface in suspensions of soft spherocylinders. 2005 , 71, 051716		40
978	Prediction of high-pressure adsorption equilibrium of supercritical gases using density functional theory. 2005 , 21, 3187-97		50
977	Computer simulations on the gas-liquid phase diagram of Stockmayer fluids. 2005 , 50, 1595		1
976	Liquid-vapor equilibrium and surface tension of nonconformal molecular fluids. <i>Journal of Chemical Physics</i> , 2005 , 122, 34504	3-9	7
975	Reactive Monte Carlo and grand-canonical Monte Carlo simulations of the propene metathesis reaction system. <i>Journal of Chemical Physics</i> , 2005 , 122, 164705	3-9	43
974	Liquid-liquid phase transitions in supercooled water studied by computer simulations of various water models. <i>Journal of Chemical Physics</i> , 2005 , 123, 044515	3-9	141
973	Effects of conformational distributions on sigma profiles in COSMO theories. 2005 , 109, 11285-94		22
972	Simulating the vapour-liquid equilibria of large cyclic alkanes. <i>Molecular Physics</i> , 2005 , 103, 99-104	1-7	31
971	A molecular-dynamics simulation study on the dependence of Lennard-Jones gas-liquid phase diagram on the long-range part of the interactions. <i>Journal of Chemical Physics</i> , 2005 , 123, 234502	3-9	24

970	Solubility of carbon dioxide in aqueous solutions of methanol. Predictions by molecular simulation and comparison with experimental data. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 14943-9	3.4	12
969	Using arbitrary trial distributions to improve intramolecular sampling in configurational-bias Monte Carlo. <i>Molecular Physics</i> , 2006 , 104, 2439-2456	1.7	47
968	Liquid-vapour equilibrium of n -alkanes using interface simulations. <i>Molecular Physics</i> , 2006 , 104, 2413-2424	3.4	35
967	Interactions of nitrous oxide with fluorinated liquids. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 18566-73	3.4	8
966	Vapor-liquid equilibria from the triple point up to the critical point for the new generation of TIP4P-like models: TIP4P/Ew, TIP4P/2005, and TIP4P/ice. <i>Journal of Chemical Physics</i> , 2006 , 125, 34503	3.9	175
965	Ornstein-Zernike equations for highly asymmetric mixtures: confronting the no-solution challenge. <i>Molecular Physics</i> , 2006 , 104, 3419-3424	1.7	3
964	Critical properties of aluminum. 2006 , 128, 4224-5		34
963	Capillary phase transitions of linear and branched alkanes in carbon nanotubes from molecular simulation. 2006 , 22, 7391-9		26
962	Statistical mechanics of nucleation: incorporating translational and rotational free energy into thermodynamics of a microdroplet. 2006 , 73, 031607		18
961	Four phases of amorphous water: Simulations versus experiment. <i>Journal of Chemical Physics</i> , 2006 , 124, 164505	3.9	20
960	Monte Carlo Simulation Study of Water Adsorption in Activated Carbon. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 5649-5656	3.9	69
959	Calculation of phase coexistence properties and surface tensions of n-alkanes with grand-canonical transition-matrix monte carlo simulation and finite-size scaling. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 1369-76	3.4	87
958	The melting point of ice Ih for common water models calculated from direct coexistence of the solid-liquid interface. <i>Journal of Chemical Physics</i> , 2006 , 124, 144506	3.9	320
957	Phase behavior of elemental aluminum using monte carlo simulations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 26135-42	3.4	15
956	A general perturbation approach for equation of state development: applications to simple fluids, ab initio potentials, and fullerenes. <i>Journal of Chemical Physics</i> , 2006 , 124, 154505	3.9	56
955	Phase equilibria in carbon dioxide expanded solvents: Experiments and molecular simulations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 13195-202	3.4	52
954	Simulation of the density of states in isothermal and adiabatic ensembles. 2006 , 73, 056701		10
953	Molecular dynamics simulation of Henry's constant of argon, nitrogen, methane and oxygen in ethylene oxide. 2006 , 32, 11-16		19

952	A study of Wertheim's thermodynamic perturbation theory (TPT1) for associating fluids with dispersive interactions: the importance of the association range. <i>Molecular Physics</i> , 2006 , 104, 3551-3560 ¹⁻⁷	12
951	Critical point estimation of the Lennard-Jones pure fluid and binary mixtures. <i>Journal of Chemical Physics</i> , 2006 , 125, 054515	3-9 76
950	Simulation study of methanol and ethanol adsorption on graphitized carbon black. 2006 , 32, 887-899	28
949	Monte Carlo simulations of CO ₂ -expanded acetonitrile. <i>Molecular Physics</i> , 2006 , 104, 2955-2960	1-7 9
948	Probing the nucleation mechanism for the binary n-nonane/1-alcohol series with atomistic simulations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 18619-28	3-4 22
947	Tracing the critical loci of binary fluid mixtures using molecular simulation. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 17200-6	3-4 8
946	Simulating fluid-phase equilibria of water from first principles. 2006 , 110, 640-6	125
945	Low-temperature vapor-liquid equilibria from parallelized molecular dynamics simulations. Application to 1- and 2-methylnaphthalene. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 12083-8	3-4
944	Simulating the vapour-liquid equilibria of 1,4-dioxane. 2006 , 32, 657-662	8
943	Monte carlo simulation of carboxylic acid phase equilibria. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 21938-43	3-4 21
942	Monte Carlo study of supramolecular polymer fractionation: selective removal of chain stoppers by phase separation. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 18629-34	3-4 5
941	Monte Carlo Calculations for the Solid-State Properties of Warfarin Sodium 2-Propanol Solvate. 2006 , 6, 1318-1323	7
940	Corresponding-states laws for protein solutions. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 17638-44	3-4 19
939	Adsorption of carbon tetrachloride on graphitized thermal carbon black and in slit graphitic pores: five-site versus one-site potential models. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 9520-8	3-4 27
938	Triangle of liquid-gas states. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 8474-80	3-4 38
937	Structure and dynamics of the aqueous liquid-vapor interface: a comprehensive particle-based simulation study. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3738-46	3-4 106
936	Molecular simulation of the adsorption of MTBE in silicalite, mordenite, and zeolite beta. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 14458-62	3-4 31
935	Direct calculation of solid-vapor coexistence points by thermodynamic integration: application to single component and binary systems. <i>Journal of Chemical Physics</i> , 2006 , 124, 184106	3-9 3

934	Applications of Molecular Simulation in Oil and Gas Production and Processing. 2006 , 61, 387-403		38
933	Vapor-liquid equilibria of water from first principles: comparison of density functionals and basis sets. <i>Molecular Physics</i> , 2006 , 104, 3619-3626	1.7	75
932	The adsorption of water in finite carbon pores. <i>Molecular Physics</i> , 2006 , 104, 623-637	1.7	22
931	Vapor-liquid phase equilibria for mixtures containing diatomic Lennard-Jones molecules. <i>Fluid Phase Equilibria</i> , 2006 , 241, 175-185	2.5	9
930	Comparison of the AMBER, CHARMM, COMPASS, GROMOS, OPLS, TraPPE and UFF force fields for prediction of vapor-liquid coexistence curves and liquid densities. <i>Fluid Phase Equilibria</i> , 2006 , 248, 50-55 ^{2.5}		102
929	Molecular simulation of structure and thermodynamic properties of pure tri- and tetra-ethylene glycols and their aqueous mixtures. <i>Fluid Phase Equilibria</i> , 2006 , 248, 134-146	2.5	11
928	Retention in gas-liquid chromatography with a polyethylene oxide stationary phase: molecular simulation and experiment. 2006 , 1126, 373-80		6
927	Isothermal-isobaric Monte Carlo simulations of liquid lithium using density functional theory. 2006 , 417, 283-287		5
926	Isotropic-nematic transition in liquid crystals confined between rough walls. 2006 , 418, 392-396		17
925	Critical point of 1D square-well fluid. 2006 , 127, 47-49		1
924	Effects of confinement on freezing and melting. <i>Journal of Physics Condensed Matter</i> , 2006 , 18, R15-68	1.8	546
923	Universal triangle of states for liquid and vapor. 2006 , 47, S109-S118		1
922	Direct calculation of Henry's law constants from Gibbs ensemble Monte Carlo simulations: nitrogen, oxygen, carbon dioxide and methane in ethanol. 2006 , 115, 391-397		75
921	Monte Carlo predictions for the phase behavior of H ₂ S+n-alkane, H ₂ S+CO ₂ , CO ₂ +CH ₄ and H ₂ S+CO ₂ +CH ₄ mixtures. <i>Fluid Phase Equilibria</i> , 2006 , 246, 71-78	2.5	19
920	Vapour-liquid equilibria of the two- and three-dimensional monoatomic classical fluids interacting via double Yukawa potential. 2006 , 67, 1141-1154		2
919	Percolating networks and liquid-liquid transitions in supercooled water. <i>Journal of Physics Condensed Matter</i> , 2006 , 18, S2247-S2259	1.8	23
918	Limitations of the rigid planar nonpolarizable models of water. <i>Journal of Chemical Physics</i> , 2006 , 124, 74507	3.9	23
917	Accelerating molecular simulations by reversible mapping between local minima. <i>Journal of Chemical Physics</i> , 2006 , 125, 084107	3.9	13

916	Computational studies on thermodynamic properties, effective diameters, and free volume of argon using an ab initio potential. <i>Journal of Chemical Physics</i> , 2006 , 125, 084510	3.9	23
915	Computing the starting state for Gibbs-Duhem integration. <i>Journal of Chemical Physics</i> , 2006 , 124, 054905	3.9	4
914	An advanced Gibbs-Duhem integration method: theory and applications. <i>Journal of Chemical Physics</i> , 2006 , 124, 054906	3.9	9
913	Liquid-vapor isotopic fractionation factors of diatomic fluids: a direct comparison between molecular simulation and experiment. <i>Journal of Chemical Physics</i> , 2006 , 125, 34510	3.9	5
912	Influence of surface chemical heterogeneities on adsorption/desorption hysteresis and coexistence diagram of metastable states within cylindrical pores. <i>Journal of Chemical Physics</i> , 2006 , 125, 074707	3.9	22
911	Phase equilibria and plate-fluid interfacial tensions for associating hard sphere fluids confined in slit pores. <i>Journal of Chemical Physics</i> , 2006 , 125, 084716	3.9	16
910	Theoretical and computational investigations on thermodynamic properties, effective site diameters, and molecular free volume of carbon disulfide fluid. <i>Journal of Chemical Physics</i> , 2006 , 125, 154505	3.9	6
909	Cluster pair correlation function of simple fluids: energetic connectivity criteria. <i>Journal of Chemical Physics</i> , 2006 , 125, 194512	3.9	4
908	Combining reactive and configurational-bias Monte Carlo: confinement influence on the propene metathesis reaction system in various zeolites. <i>Journal of Chemical Physics</i> , 2006 , 125, 224709	3.9	37
907	Direct determination of liquid phase coexistence by Monte Carlo simulations. 2006 , 74, 016111		3
906	Simulation of phase transitions in highly asymmetric fluid mixtures. 2006 , 97, 115705		15
905	Critical comparison of classical and quantum mechanical treatments of the phase equilibria of water. <i>Journal of Chemical Physics</i> , 2006 , 124, 114505	3.9	8
904	Development of a new polarizable potential model of hydrogen fluoride and comparison with other effective models in liquid and supercritical states. <i>Journal of Chemical Physics</i> , 2006 , 124, 184504	3.9	7
903	Nonequilibrium anisotropic phases, nucleation, and critical behavior in a driven Lennard-Jones fluid. 2006 , 73,		3
902	Analysis of gas adsorption in Kureha active carbon based on the slit-pore model and Monte-Carlo simulations. 2006 , 32, 513-522		8
901	Phase behavior and structure of model colloid-polymer mixtures confined between two parallel planar walls. 2006 , 73, 051502		39
900	Simulation study of ammonia adsorption on graphitized carbon black. 2006 , 32, 523-537		9
899	Multiple extrema in the intermolecular potential and the phase diagram of protein solutions. 2006 , 73, 061917		18

898	Simple model of membrane proteins including solvent. <i>Journal of Chemical Physics</i> , 2006 , 124, 184904	3.9	2
897	Reactive Canonical Monte Carlo. <i>Advances in Chemical Physics</i> , 2007 , 461-481		14
896	Semigrand Canonical Monte Carlo Simulation; Integration Along Coexistence Lines. <i>Advances in Chemical Physics</i> , 2007 , 405-441		33
895	Thermodynamic-Scaling Methods in Monte Carlo and their Application to Phase Equilibria. <i>Advances in Chemical Physics</i> , 2007 , 369-404		7
894	An Introduction to the Monte Carlo Method for Particle Simulations. <i>Advances in Chemical Physics</i> , 2007 , 1-12		4
893	Computational study of the melting-freezing transition in the quantum hard-sphere system for intermediate densities. II. Structural features. <i>Journal of Chemical Physics</i> , 2007 , 126, 164509	3.9	6
892	Non-Hamiltonian molecular dynamics implementation of the Gibbs ensemble method. I. Algorithm. <i>Journal of Chemical Physics</i> , 2007 , 126, 164104	3.9	6
891	Non-Hamiltonian molecular dynamics implementation of the Gibbs ensemble method. II. Molecular liquid-vapor results for carbon dioxide. <i>Journal of Chemical Physics</i> , 2007 , 126, 164105	3.9	12
890	Effect of confinement on the liquid-liquid phase transition of supercooled water. <i>Journal of Chemical Physics</i> , 2007 , 126, 214701	3.9	32
889	Phase diagram of model anisotropic particles with octahedral symmetry. <i>Journal of Chemical Physics</i> , 2007 , 127, 054501	3.9	76
888	Regarding convergence curve of virial expansion for the Lennard-Jones system. <i>Journal of Chemical Physics</i> , 2007 , 127, 064507	3.9	13
887	Phase diagram for a model of urate oxidase. <i>Journal of Chemical Physics</i> , 2007 , 127, 165105	3.9	1
886	Effect of packing parameter on phase diagram of amphiphiles: an off-lattice Gibbs ensemble approach. <i>Journal of Chemical Physics</i> , 2007 , 127, 244905	3.9	5
885	Formation of rodlike structures of water between oppositely charged ions in decane and polyethylene. <i>Journal of Chemical Physics</i> , 2007 , 127, 191101	3.9	2
884	Optimized expanded ensembles for simulations involving molecular insertions and deletions. II. Open systems. <i>Journal of Chemical Physics</i> , 2007 , 127, 174104	3.9	24
883	Thermodynamic properties for the triangular-well fluid. <i>Molecular Physics</i> , 2007 , 105, 2987-2998	1.7	23
882	Computational study of the melting-freezing transition in the quantum hard-sphere system for intermediate densities. I. Thermodynamic results. <i>Journal of Chemical Physics</i> , 2007 , 126, 164508	3.9	13
881	Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene. <i>Journal of Chemical Physics</i> , 2007 , 126, 224902	3.9	21

880	Effective critical point location: application to thiophenes. 2007 , 33, 777-785		6
879	Water absorption in polyethylene under external electric fields. <i>Journal of Chemical Physics</i> , 2007 , 127, 024902	3.9	1
878	Phase separation of charge-stabilized colloids: a Gibbs ensemble Monte Carlo simulation study. 2007 , 75, 061403		14
877	On the heat capacity of adsorbed phases using molecular simulation. <i>Journal of Chemical Physics</i> , 2007 , 126, 064702	3.9	3
876	Ehrenfest urn revisited: playing the game on a realistic fluid model. 2007 , 76, 011104		4
875	Water-like solvation thermodynamics in a spherically symmetric solvent model with two characteristic lengths. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 20177-82	11.5	90
874	Surface tension and vapor-liquid phase coexistence of confined square-well fluid. <i>Journal of Chemical Physics</i> , 2007 , 126, 024702	3.9	58
873	Criticality of Ionic Fluids. <i>Advances in Chemical Physics</i> , 2007 , 1-66		54
872	Molecular-Based Modeling of Water and Aqueous Solutions at Supercritical Conditions. <i>Advances in Chemical Physics</i> , 2007 , 115-205		51
871	The Monte Carlo method. 295-337		
870	Classical equilibrium statistical mechanics. 169-196		
869	Liquid-vapour transition of the long range Yukawa fluid. <i>Molecular Physics</i> , 2007 , 105, 1813-1826	1.7	19
868	Gas-liquid phase coexistence in a tetrahedral patchy particle model. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 322101	1.8	27
867	Effect of pore morphology and topology on capillary condensation in nanopores: a theoretical and molecular simulation study. 2007 , 160, 1-8		10
866	Transferable potentials for phase equilibria. 9. Explicit hydrogen description of benzene and five-membered and six-membered heterocyclic aromatic compounds. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 10790-9	3.4	162
865	Anisotropic United Atom Model Including the Electrostatic Interactions of Methylbenzenes. I. Thermodynamic and Structural Properties. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 15686-15699	3.8	46
864	Molecular simulations of the n-alkane liquid-vapor interface: interfacial properties and their long range corrections. 2007 , 75, 051602		94
863	Free Energy Calculations. 2007 ,		592

862	Water in Nanopores: III. Surface Phase Transitions of Water on Hydrophilic Surfaces□ <i>Journal of Physical Chemistry C</i> , 2007 , 111, 15716-15725	3.8	22
861	Phase diagrams of alkali halides using two interaction models: a molecular dynamics and free energy study. <i>Journal of Chemical Physics</i> , 2007 , 126, 024503	3.9	20
860	Spatial correlation of dipole fluctuations in liquid water. <i>Molecular Physics</i> , 2007 , 105, 1411-1417	1.7	22
859	Adsorption of normal pentane on the surface of rutile. Experimental results and simulations. 2007 , 23, 7555-61		6
858	Prediction of phase equilibria and transport properties in carbon-dioxide expanded solvents by molecular simulation. 2007 , 33, 861-869		25
857	A molecular simulation approach to the study of adsorption of hydrogen cyanide and methyl ethyl ketone in silicalite, mordenite and zeolite beta structures. 2007 , 33, 843-850		10
856	Energetics and volume changes in electron attachment to pyrazine in supercritical xenon. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 6684-9	3.4	6
855	Structure and thermodynamics of discrete potential fluids in the OZEMSA formalism. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 086224	1.8	9
854	Computational Approaches in Molecular Recognition, Self-assembly, Electron Transport, and Surface Chemistry. 2007 , 19, 229-241		9
853	Results from an Early Polarization Model Based on Maxwell's Invariant Multipole Form. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 2138-45	6.4	3
852	Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends. 2007 , 40, 2904-2914		8
851	Pressure Dependence of the Hildebrand Solubility Parameter and the Internal Pressure: Monte Carlo Simulations for External Pressures up to 300 MPa□ <i>Journal of Physical Chemistry C</i> , 2007 , 111, 15634-15641	3.8	40
850	An anisotropic united atoms (AUA) potential for thiophenes. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 4460-6	3.4	21
849	Applications of Wang-Landau sampling to determine phase equilibria in complex fluids. <i>Journal of Chemical Physics</i> , 2007 , 127, 154504	3.9	79
848	Molecular Dynamics Simulation of Sorption of Gases in Polystyrene. 2007 , 40, 6413-6421		60
847	Hard Convex Body Fluids. <i>Advances in Chemical Physics</i> , 2007 , 1-166		179
846	Computational Physics. 2007 ,		113
845	Thermodynamic and transport properties of carbon dioxide from molecular simulation. <i>Journal of Chemical Physics</i> , 2007 , 126, 064509	3.9	64

844	Simulation Study of Water Adsorption on Carbon Black: The Effect of Graphite Water Interaction Strength. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 5735-5742	3.8	41
843	Anisotropic united atom model including the electrostatic interactions of benzene. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 3730-41	3.4	38
842	Revisiting the Frenkel-Ladd method to compute the free energy of solids: the Einstein molecule approach. <i>Journal of Chemical Physics</i> , 2007 , 127, 154113	3.9	124
841	Molecular simulation applied to fluid properties in the oil and gas industry. 2007 , 33, 287-304		33
840	Dependence of the critical temperature on molecular parameters. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 5941-5	3.4	8
839	References. 329-360		
838	Prediction of viscosities and vapor-liquid equilibria for five polyhydric alcohols by molecular simulation. <i>Fluid Phase Equilibria</i> , 2007 , 260, 218-231	2.5	58
837	Prediction of the bubble point pressure for the binary mixture of ethanol and 1,1,1,2,3,3,3-heptafluoropropane from Gibbs ensemble Monte Carlo simulations using the TraPPE force field. <i>Fluid Phase Equilibria</i> , 2007 , 260, 199-211	2.5	11
836	New force fields for nitrous oxide and oxygen and their application to phase equilibria simulations. <i>Fluid Phase Equilibria</i> , 2007 , 259, 180-188	2.5	40
835	Validation of the COSMO-RS electrostatics by Monte-Carlo simulations. <i>Fluid Phase Equilibria</i> , 2007 , 261, 162-167	2.5	5
834	Solid-liquid phase equilibria for mixtures containing diatomic Lennard-Jones molecules. <i>Fluid Phase Equilibria</i> , 2007 , 262, 1-13	2.5	7
833	Molecular simulation of the thermophysical properties of fluids: From understanding toward quantitative predictions. 2007 , 134, 71-89		78
832	Testing the adequacy of simple water models at the opposite ends of the phase diagram. 2007 , 134, 94-98		7
831	Introduction. 2007 , 1-31		4
830	Retention mechanism in reversed-phase liquid chromatography: a molecular perspective. 2007 , 79, 6551-8		117
829	Simplified gauge-cell method and its application to the study of capillary phase transition of propane in carbon nanotubes. 2007 , 13, 21-32		15
828	Hydrogen/hydrocarbon phase equilibrium modelling with a cubic equation of state and a Monte Carlo method. <i>Fluid Phase Equilibria</i> , 2007 , 254, 211-223	2.5	19
827	Molecular simulation of the solubility and diffusion of carbon dioxide and hydrogen sulfide in polyethylene melts. <i>Fluid Phase Equilibria</i> , 2007 , 261, 168-175	2.5	28

826	Bubble point pressure estimates from Gibbs ensemble simulations. <i>Fluid Phase Equilibria</i> , 2007 , 260, 195-198	2.5	11
825	Molecular dynamics study on the phase diagrams of linear and branched chain molecules. 2008 , 344, 52-60		2
824	Equation of state for the Lennard-Jones fluid based on the perturbation theory. <i>Fluid Phase Equilibria</i> , 2008 , 264, 174-183	2.5	18
823	Optimized intermolecular potential for nitriles based on Anisotropic United Atoms model. 2008 , 14, 571-80		5
822	Phase Equilibria and Plate-fluid Interfacial Tensions for Four-site Associating Lennard-Jones Fluids Confined in Slit Pores. 2008 , 26, 269-275		
821	Improvement in molecule exchange efficiency in Gibbs ensemble Monte Carlo: development and implementation of the continuous fractional component move. 2008 , 29, 2520-30		81
820	Simulation of the (vapor + liquid) equilibria of binary mixtures of benzene, cyclohexane, and hydrogen. 2008 , 40, 271-283		7
819	Molecular simulation of the effect of ionic impurities and external electric fields on rod-like water clusters in polyethylene. 2008 , 49, 5357-5362		5
818	Two-dimensional chiral segregation of the bent hard needles model with Lennard-Jones sites. 2008 , 387, 145-158		7
817	Economic simplex optimization for broad range property prediction: Strengths and weaknesses of an automated approach for tailoring of parameters. <i>Fluid Phase Equilibria</i> , 2008 , 274, 27-35	2.5	10
816	Molecular-level simulations of chemical reaction equilibrium for nitric oxide dimerization reaction in disordered nanoporous carbons. <i>Fluid Phase Equilibria</i> , 2008 , 272, 18-31	2.5	14
815	Development of the TraPPE-UA force field for ethylene oxide. <i>Fluid Phase Equilibria</i> , 2008 , 274, 44-49	2.5	27
814	Simulation of chemical reaction equilibria by the reaction ensemble Monte Carlo method: a review 2008 , 34, 119-146		90
813	Spherically averaged versus angle-dependent interactions in quadrupolar fluids. 2008 , 77, 041506		21
812	Monte Carlo simulations of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB): Pressure and temperature effects for the solid phase and vapor-liquid phase equilibria. <i>Journal of Chemical Physics</i> , 2008 , 129, 194510	3.0	34
811	Handling Electrostatic Interactions in Molecular Simulations: A Systematic Study. 2008 , 73, 481-506		13
810	Determination of phase diagrams via computer simulation: methodology and applications to water, electrolytes and proteins. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 153101	1.8	180
809	Solubility in supercritical carbon dioxide: importance of the Poynting correction and entrainer effects. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 11374-80	3.4	34

808	Population Inversion of a NAHS Mixture Adsorbed into a Cylindrical Pore. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 18028-18033	3.8	15
807	Molecular simulations of zeolites: adsorption, diffusion, and shape selectivity. 2008 , 108, 4125-84		564
806	Simulations of phase transitions and free energies for ionic systems. <i>Molecular Physics</i> , 2008 , 106, 2039-2051	3.6	
805	Application of the TraPPE Force Field for Predicting the Hildebrand Solubility Parameters of Organic Solvents and Monomer Units. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 136-44	6.4	26
804	Structure of the Methanol Liquid/Vapor Interface: A Comprehensive Particle-Based Simulation Study. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 15412-15418	3.8	21
803	Theoretical and numerical study of the phase diagram of patchy colloids: ordered and disordered patch arrangements. <i>Journal of Chemical Physics</i> , 2008 , 128, 144504	3.9	134
802	Surface tensions of linear and branched alkanes from Monte Carlo simulations using the anisotropic united atom model. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 13885-97	3.4	45
801	Comparing the Use of Gibbs Ensemble and Grand-Canonical Transition-Matrix Monte Carlo Methods to Determine Phase Equilibria. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 4533-4541	3.9	49
800	An optimised molecular model for ammonia. <i>Molecular Physics</i> , 2008 , 106, 1039-1046	1.7	39
799	Vapour/Liquid equilibrium of fluids composed by oblate molecules. <i>Molecular Physics</i> , 2008 , 106, 1331-1339	3.7	13
798	Confinement effects on phase behavior of soft matter systems. 2008 , 4, 1555-1568		108
797	Monte Carlo simulations of thermodynamic and structural properties of Mie(14,7) fluids. <i>Journal of Chemical Physics</i> , 2008 , 128, 154514	3.9	19
796	The phase diagram of the Lennard-Jones fluid using temperature dependent interaction parameters. 2008 , 34, 289-294		12
795	Optimisation of the dynamical behaviour of the anisotropic united atom model of branched alkanes: application to the molecular simulation of fuel gasoline. 2008 , 34, 211-230		17
794	Thermodynamics of a long-range triangle-well fluid. <i>Molecular Physics</i> , 2008 , 106, 113-126	1.7	28
793	Thermodynamic behavior of the CO ₂ + NO ₂ /N ₂ O ₄ mixture: a Monte Carlo simulation study. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 15783-92	3.4	21
792	Expressions for local contributions to the surface tension from the virial route. 2008 , 77, 031601		63
791	A New United Atom Force Field for Adsorption of Alkenes in Zeolites. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 2492-2498	3.8	55

790	Size Effects on the Solvation of Anions at the Aqueous Liquid-Vapor Interface. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 210-218	3.8	63
789	An aggregation-volume-bias Monte Carlo investigation on the condensation of a Lennard-Jones vapor below the triple point and crystal nucleation in cluster systems: an in-depth evaluation of the classical nucleation theory. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 4067-78	3.4	44
788	Studies of the thermodynamic properties of hydrogen gas in bulk water. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 867-76	3.4	36
787	Influence of the displacement out of the center of mass and nonaxiality of the dipole on the thermodynamics of liquids composed of linear dipole molecules. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 8069-75	3.4	6
786	Monte Carlo and Molecular Dynamics. 2008 , 77-101		1
785	Continuum percolation of long lifespan clusters in a simple fluid. <i>Journal of Chemical Physics</i> , 2008 , 129, 064510	3.9	5
784	Surface tension of water and acid gases from Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2008 , 128, 154716	3.9	76
783	Nanocomposites. 2008 ,		15
782	Efficient prediction of thermodynamic properties of quadrupolar fluids from simulation of a coarse-grained model: the case of carbon dioxide. <i>Journal of Chemical Physics</i> , 2008 , 128, 104501	3.9	44
781	Phase behavior of semiflexible polymer chains. <i>Journal of Chemical Physics</i> , 2008 , 128, 124908	3.9	14
780	Multiple histogram reweighting method for the surface tension calculation. <i>Journal of Chemical Physics</i> , 2008 , 128, 154718	3.9	40
779	Effect of flexibility on surface tension and coexisting densities of water. <i>Journal of Chemical Physics</i> , 2008 , 128, 174703	3.9	47
778	Role of solvent in protein phase behavior: Influence of temperature dependent potential. <i>Journal of Chemical Physics</i> , 2008 , 128, 235104	3.9	11
777	Phase diagram of a model of nanoparticles in electrolyte solutions. <i>Journal of Chemical Physics</i> , 2008 , 129, 164113	3.9	4
776	Fluid phase behavior of a model colloid-polymer mixture: Influence of polymer size and interaction strength. <i>Journal of Chemical Physics</i> , 2008 , 129, 164907	3.9	14
775	Theory and atomistic simulation of krypton fluid. <i>Journal of Chemical Physics</i> , 2008 , 129, 244504	3.9	4
774	Hofmeister effect and the phase diagram of lysozyme. 2008 , 78, 011921		3
773	The self-referential method combined with thermodynamic integration. <i>Journal of Chemical Physics</i> , 2008 , 128, 064102	3.9	8

772	Comment on "An optimized potential for carbon dioxide" [J. Chem. Phys. 122, 214507 (2005)]. <i>Journal of Chemical Physics</i> , 2008 , 129, 087101; author reply 087102	3.9	14
771	Effects due to molecular shape and flexibility on the permeability ratio of binary fluid mixtures in a model polymer network via computer simulation. <i>Journal of Chemical Physics</i> , 2008 , 128, 084902	3.9	1
770	Polymer-induced phase separation and crystallization in immunoglobulin G solutions. <i>Journal of Chemical Physics</i> , 2008 , 128, 205105	3.9	11
769	Phase diagram of Janus particles. 2009 , 103, 237801		227
768	Structural relaxation of a gel modeled by three body interactions. 2009 , 103, 248305		30
767	Freezing parameters of soft spheres. <i>Molecular Physics</i> , 2009 , 107, 295-299	1.7	8
766	Ion specific effects on phase transitions in protein solutions. 2009 , 79, 031904		5
765	Nucleation in a Potts lattice gas model of crystallization from solution. <i>Journal of Chemical Physics</i> , 2009 , 131, 184101	3.9	47
764	TIGER2: an improved algorithm for temperature intervals with global exchange of replicas. <i>Journal of Chemical Physics</i> , 2009 , 130, 174106	3.9	40
763	Simulation of water clusters in vapour, alkanes and polyethylenes. 2009 , 35, 888-896		6
762	Phase equilibrium of colloidal suspensions with particle size dispersity: a Monte Carlo study. <i>Journal of Chemical Physics</i> , 2009 , 130, 194902	3.9	10
761	New techniques for simulating crystals. 2009 , 35, 897-909		5
760	Self-diffusion coefficient of two-center Lennard-Jones fluids: molecular simulations and free volume theory. <i>Journal of Chemical Physics</i> , 2009 , 130, 024503	3.9	10
759	Influence of reservoir size on the adsorption path in an ideal pore. <i>Journal of Chemical Physics</i> , 2009 , 131, 124123	3.9	20
758	Effect of the interfacial area on the equilibrium properties of Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 2009 , 131, 124513	3.9	24
757	Additive and nonadditive models of vapor-liquid equilibrium in CO ₂ from first principles. <i>Journal of Chemical Physics</i> , 2009 , 130, 034110	3.9	30
756	From discovery to data: What must happen for molecular simulation to become a mainstream chemical engineering tool. 2009 , 55, 1304-1310		59
755	Accurate thermodynamic and dielectric equations of state for high-temperature simulated water. <i>Fluid Phase Equilibria</i> , 2009 , 277, 145-151	2.5	28

754	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability. Theory and applications. 2009 , 124, 11-28		285
753	Molecular dynamics simulation of liquid-vapor phase equilibria in polar fluids. 2009 , 473, 66-71		10
752	Vapor-liquid phase equilibria of water modelled by a Kim-Gordon potential. 2009 , 479, 60-64		2
751	Calculation of the surface tension of cyclic and aromatic hydrocarbons from Monte Carlo simulations using an anisotropic united atom model (AUA). 2009 , 11, 6132-47		30
750	Solid-liquid phase equilibria of the Gaussian core model fluid. <i>Journal of Chemical Physics</i> , 2009 , 131, 184507	3.9	14
749	Monte Carlo simulations of the pressure dependence of the water-acid gas interfacial tensions. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 14277-90	3.4	53
748	Role of the range in the fluid-crystal coexistence for a patchy particle model. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 15133-6	3.4	45
747	Transferable force field for alcohols and polyalcohols. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 5985-95	3.4	60
746	All-atom force field for the prediction of vapor-liquid equilibria and interfacial properties of HFA134a. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 178-87	3.4	34
745	TrAPPE-UA force field for acrylates and Monte Carlo simulations for their mixtures with alkanes and alcohols. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 6415-25	3.4	69
744	Adsorption and Diffusion of Light Gases in ZIF-68 and ZIF-70: A Simulation Study. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 16906-16914	3.8	118
743	Phase behavior in suspensions of highly charged colloids. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 6766-74	3.4	16
742	Exploring the formation of multiple layer hydrates for a complex pharmaceutical compound. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 5929-37	3.4	12
741	Computer simulation of volatile organic compound adsorption in atomistic models of molecularly imprinted polymers. 2009 , 25, 5352-9		60
740	Volumetric Properties of Hydration Water. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 11110-11118	3.8	9
739	Virial coefficients of Lennard-Jones mixtures. <i>Journal of Chemical Physics</i> , 2009 , 130, 224104	3.9	14
738	Coarse-grained models for fluids and their mixtures: Comparison of Monte Carlo studies of their phase behavior with perturbation theory and experiment. <i>Journal of Chemical Physics</i> , 2009 , 130, 044103	3.9	49
737	Phase equilibria of molecular fluids via hybrid Monte Carlo Wang-Landau simulations: applications to benzene and n-alkanes. <i>Journal of Chemical Physics</i> , 2009 , 130, 244109	3.9	50

736	Solubility of CO ₂ in (Water + Acetone): Correlation of Experimental Data and Predictions from Molecular Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 4553-4564	3.9	9
735	Liquid-vapor equilibrium isotopic fractionation of water: how well can classical water models predict it?. <i>Journal of Chemical Physics</i> , 2009 , 130, 094509	3.9	14
734	Thermodynamics and Kinetics of Nanoclusters Controlling Gas-to-Particle Nucleation. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 10354-10370	3.8	51
733	Water permeability of poly(ethylene terephthalate): a grand canonical ensemble molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2009 , 131, 234904	3.9	20
732	Vapour-liquid phase transition of dipolar particles. <i>Molecular Physics</i> , 2009 , 107, 403-413	1.7	45
731	Monte-Carlo multiscale simulation study of argon adsorption/desorption hysteresis in mesoporous heterogeneous tubular pores like MCM-41 or oxidized porous silicon. 2009 , 25, 903-11		43
730	Microscopic structure and interaction analysis for supercritical carbon dioxide-ethanol mixtures: a Monte Carlo simulation study. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 4781-9	3.4	27
729	Critical behavior of soft matter fluids in bulk and in random porous media: from Ising to random-field Ising universality. 2009 , 5, 4388		16
728	Coarse-graining dipolar interactions in simple fluids and polymer solutions: Monte Carlo studies of the phase behavior. 2009 , 11, 1923-33		10
727	Temperature accelerated dynamics in glass-forming materials. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 7844-53	3.4	8
726	First principles models of the interactions of methane and carbon dioxide. <i>Fluid Phase Equilibria</i> , 2010 , 290, 48-54	2.5	15
725	Monte Carlo Simulation of Vapor-liquid Equilibria for Perfluoropropane (R-218) and 2,3,3,3-Tetrafluoropropene (R-1234yf). 2010 , 31, 462-474		6
724	Specific ion effects and the phase diagram of lysozyme. 2010 , 6, 46-51		
723	Molecular simulations of benzene and hexafluorobenzene using new optimized effective potential models: Investigation of the liquid, vapor-liquid coexistence and supercritical fluid phases. 2010 , 153, 25-30		6
722	Molecular force field investigation for Sulfur Hexafluoride: A computer simulation study. <i>Fluid Phase Equilibria</i> , 2010 , 291, 81-89	2.5	29
721	Monte Carlo simulations of vapor-liquid-liquid equilibrium of some ternary petrochemical mixtures. <i>Fluid Phase Equilibria</i> , 2010 , 299, 24-31	2.5	4
720	Ethanoled gasoline bubble pressure determination: Experimental and Monte Carlo modeling. <i>Fluid Phase Equilibria</i> , 2010 , 299, 132-140	2.5	11
719	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. 2010 , 55, 503-509		5

718	The Linked Neighbour List (LNL) method for fast off-lattice Monte Carlo simulations of fluids. 2010 , 181, 569-581		2
717	Vapor-Liquid equilibria of copper using hybrid Monte Carlo Wang-Landau simulations. <i>Fluid Phase Equilibria</i> , 2010 , 287, 79-83	2.5	42
716	Adsorption and Phase Behaviour in Nanochannels and Nanotubes. 2010 ,		20
715	Field-theoretic simulations in the Gibbs ensemble. <i>Journal of Chemical Physics</i> , 2010 , 132, 024104	3.9	37
714	Coexistence curves in monatomic fluids: the contrast between insulating argon and metallic assemblies. 2010 , 48, 561-563		
713	Gibbs ensemble Monte Carlo simulations of binary vapour-liquid equilibrium: application to n-hexane-water and ethane-ethanol systems. 2010 , 36, 758-762		5
712	Phase diagram of a tetrahedral patchy particle model for different interaction ranges. <i>Journal of Chemical Physics</i> , 2010 , 132, 184501	3.9	102
711	Equilibrium self-assembly of colloids with distinct interaction sites: thermodynamics, percolation, and cluster distribution functions. <i>Journal of Chemical Physics</i> , 2010 , 132, 234502	3.9	42
710	Multi-objective optimisation on the basis of random models for ethylene oxide. 2010 , 36, 1208-1218		5
709	Polymer Phase Separation. 2010 , 47-83		1
708	Molecular model for carbon dioxide optimized to vapor-liquid equilibria. <i>Journal of Chemical Physics</i> , 2010 , 132, 234512	3.9	53
707	A numerical test of a high-penetrability approximation for the one-dimensional penetrable-square-well model. <i>Journal of Chemical Physics</i> , 2010 , 133, 024101	3.9	14
706	Communication: Tracing phase boundaries via molecular simulation: an alternative to the Gibbs-Duhem integration method. <i>Journal of Chemical Physics</i> , 2010 , 133, 111104	3.9	15
705	Monte Carlo cluster algorithm for fluid phase transitions in highly size-asymmetrical binary mixtures. <i>Journal of Chemical Physics</i> , 2010 , 133, 194102	3.9	10
704	Fluid phase coexistence and critical behavior from simulations in the restricted Gibbs ensemble. <i>Journal of Chemical Physics</i> , 2010 , 132, 074111	3.9	8
703	Direct determination of fluid-solid coexistence of square-well fluids confined in narrow cylindrical hard pores. <i>Journal of Chemical Physics</i> , 2010 , 132, 224504	3.9	12
702	Non-existence of a phase transition for penetrable square wells in one dimension. 2010 , 2010, P07030		8
701	Phase equilibria of polyaromatic hydrocarbons by hybrid Monte Carlo Wang-Landau simulations. <i>Molecular Physics</i> , 2010 , 108, 151-158	1.7	28

700	Computer simulations of critical phenomena and phase behaviour of fluids. <i>Molecular Physics</i> , 2010 , 108, 1797-1815	1.7	22
699	Molecular Computations of Adsorption in Nanoporous Materials. 2010 , 69-100		2
698	Optimisation of multiple time-step hybrid Monte Carlo Wang-Landau simulations in the isobaric-isothermal ensemble for the determination of phase equilibria. 2010 , 36, 544-551		18
697	A numerical study of one-patch colloidal particles: from square-well to Janus. 2010 , 12, 11869-77		116
696	Computational Investigation on the Role of Plasticizers on Ion Conductivity in Poly(ethylene oxide) LiTFSI Electrolytes. 2010 , 43, 3502-3510		26
695	Gibbs ensemble Monte Carlo simulations of binary mixtures of methane, difluoromethane, and carbon dioxide. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 3879-86	3-4	15
694	Liquid-Vapor Phase Equilibria and Surface Tension of Ethane As Predicted by the TraPPE and OPLS Models 2010 , 55, 5465-5470		15
693	A force field for 3,3,3-fluoro-1-propenes, including HFO-1234yf. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 10133-42	3-4	62
692	Investigation of the local structure in sub and supercritical ammonia using the nearest neighbor approach: a molecular dynamics analysis. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 15003-10	3-4	17
691	Effects of an applied electric field on the vapor-liquid equilibria of water, methanol, and dimethyl ether. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 4261-70	3-4	34
690	Extension of a charged anisotropic united atoms model to polycyclic aromatic compounds. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 6522-30	3-4	14
689	Progress and Outlook in Monte Carlo Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 3047-3058	3-9	86
688	Monte Carlo simulations of mixtures involving ketones and aldehydes by a direct bubble pressure calculation. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 8680-8	3-4	32
687	Computer Simulations and Coarse-Grained Molecular Models Predicting the Equation of State of Polymer Solutions. 2010 , 329-387		5
686	Vapor-liquid nucleation of argon: exploration of various intermolecular potentials. <i>Journal of Chemical Physics</i> , 2010 , 133, 084106	3-9	19
685	Molecular Simulation: Can it Help in the Development of Micro and Nano Devices?. 2010 , 309-331		1
684	Melting point and phase diagram of methanol as obtained from computer simulations of the OPLS model. <i>Journal of Chemical Physics</i> , 2010 , 132, 094505	3-9	19
683	Development of the trappe force field for ammonia. 2010 , 75, 577-591		27

682	Microscopic structure of liquid 1-1-1-2-tetrafluoroethane (R134a) from Monte Carlo simulation. 2010 , 12, 13266-72		10
681	The penetrable square-well model: extensive versus non-extensive phases. <i>Molecular Physics</i> , 2011 , 109, 2723-2736	1.7	14
680	On the difference between a point multipole and an equivalent linear arrangement of point charges in force field models for vapour-liquid equilibria; partial charge based models for 59 real fluids. <i>Molecular Physics</i> , 2011 , 109, 1975-1982	1.7	11
679	The experimental liquid-vapor phase diagram of bulk nuclear matter. 2011 , 38, 113101		15
678	Phase behavior of hard colloidal platelets using free energy calculations. <i>Journal of Chemical Physics</i> , 2011 , 134, 094501	3.9	54
677	Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 69-77	3.9	23
676	Molecular simulation of the binary mixture of 1-1-1-2-tetrafluoroethane and carbon dioxide. 2011 , 13, 15708-13		4
675	Pair correlation function integrals: computation and use. <i>Journal of Chemical Physics</i> , 2011 , 135, 084113	3.9	8
674	A general and efficient Monte Carlo method for sampling intramolecular degrees of freedom of branched and cyclic molecules. <i>Journal of Chemical Physics</i> , 2011 , 135, 134121	3.9	63
673	Simple one-center model for linear molecules: application to carbon dioxide. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 10073-8	3.4	6
672	Prediction of the temperature dependence of the surface tension of SO ₂ , N ₂ , O ₂ , and Ar by Monte Carlo molecular simulations. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 9421-30	3.4	48
671	Molecular simulations of retention in chromatographic systems: use of biased Monte Carlo techniques to access multiple time and length scales. 2012 , 307, 181-200		
670	A Monte Carlo study of the freezing transition of hard spheres. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 325106	1.8	12
669	Thermodynamic properties for applications in chemical industry via classical force fields. 2012 , 307, 201-49		21
668	Phase diagram of the penetrable-square-well model. 2011 , 93, 26002		15
667	Statistical thermodynamics of fluids with both dipole and quadrupole moments. <i>Journal of Chemical Physics</i> , 2011 , 134, 234507	3.9	4
666	Entropies of Condensed Phases and Complex Systems. 2011 ,		12
665	Vapor-liquid coexistence curves for methanol and methane using dispersion-corrected density functional theory. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 11688-92	3.4	35

664	A transferable force field to predict phase equilibria and surface tension of ethers and glycol ethers. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 10654-64	3.4	43
663	Flexible or rigid molecular models? A study on vapour-liquid equilibrium properties of ammonia. <i>Molecular Physics</i> , 2011 , 109, 619-624	1.7	12
662	The role of molecular modeling in confined systems: impact and prospects. 2011 , 13, 58-85		142
661	A water-swap reaction coordinate for the calculation of absolute protein-ligand binding free energies. <i>Journal of Chemical Physics</i> , 2011 , 134, 054114	3.9	53
660	Vapor-Liquid Coexistence and Critical Behavior of Ionic Liquids via Molecular Simulations. 2011 , 2, 1439-1443		65
659	Determining force field parameters using a physically based equation of state. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 7872-80	3.4	31
658	Simulating water with rigid non-polarizable models: a general perspective. 2011 , 13, 19663-88		640
657	Monte Carlo simulations. 255-272		
656	Note on Calculation of the Pressure in a Gibbs Ensemble. 2011 , 80, 024003		4
655	Monte Carlo Molecular Simulation of Phase-coexistence for Oil Production and Processing. 2011 ,		2
654	Characterization of uncertainty in the classification of multivariate assays: application to PAM50 centroid-based genomic predictors for breast cancer treatment plans. 2011 , 1, 37		15
653	Gibbs ensemble Monte Carlo simulations for the liquid-liquid phase equilibria of dipropylene glycol dimethyl ether and water: A preliminary report. <i>Fluid Phase Equilibria</i> , 2011 , 310, 11-18	2.5	16
652	Liquid-liquid equilibria of dipropylene glycol dimethyl ether and water by molecular dynamics. <i>Fluid Phase Equilibria</i> , 2011 , 310, 25-31	2.5	10
651	The sixth industrial fluid properties simulation challenge. <i>Fluid Phase Equilibria</i> , 2011 , 310, 1-3	2.5	12
650	Replica exchange and expanded ensemble simulations as Gibbs sampling: simple improvements for enhanced mixing. <i>Journal of Chemical Physics</i> , 2011 , 135, 194110	3.9	118
649	Alcohol Adsorption onto Silicalite from Aqueous Solution. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 18659-18669	3.8	32
648	Crystallization of tetrahedral patchy particles in silico. <i>Journal of Chemical Physics</i> , 2011 , 134, 174502	3.9	99
647	Prediction of the Surface Tension of the Liquid-Vapor Interface of Alcohols from Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 8670-8683	3.8	41

646	Assessing group-based cutoffs and the Ewald method for electrostatic interactions in clusters and in saturated, superheated, and supersaturated vapor phases of dipolar molecules. 2011 , 130, 83-93		6
645	Helium solubility in uranium dioxide from molecular dynamics simulations. 2011 , 414, 83-87		11
644	Extension of the exp-6 model to the simulation of vapor-liquid equilibria of primary alcohols and their mixtures. <i>Fluid Phase Equilibria</i> , 2011 , 301, 73-79	2.5	5
643	Gas-liquid phase coexistence and finite-size effects in a two-dimensional Lennard-Jones system. 2011 , 56, 2773-2779		5
642	Prediction of thermodynamic, transport and vapor-liquid equilibrium properties of binary mixtures of ethylene glycol and water. <i>Fluid Phase Equilibria</i> , 2011 , 301, 137-144	2.5	15
641	Thermodynamic study of binary systems containing sulphur dioxide: Measurements and molecular modelling. <i>Fluid Phase Equilibria</i> , 2011 , 304, 21-34	2.5	22
640	Isothermal vapor-liquid equilibrium data for the carbon dioxide (R744)+decafluorobutane (R610) system at temperatures from 263 to 353K. <i>Fluid Phase Equilibria</i> , 2011 , 304, 44-51	2.5	25
639	Equilibration of fluid-phase coexistence in polydisperse particle systems with short- and moderate-range depletion attractions. <i>Fluid Phase Equilibria</i> , 2011 , 305, 9-18	2.5	3
638	Monte Carlo simulation of solute extraction via supercritical carbon dioxide from poly(ethylene glycol). <i>Fluid Phase Equilibria</i> , 2011 , 305, 76-82	2.5	10
637	A critical behavior of the Lennard-Jones dimeric fluid in two-dimensions.: A Monte Carlo study. 2011 , 605, 1219-1223		7
636	Crowding of polymer coils and demixing in nanoparticle-polymer mixtures. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 285102	1.8	18
635	Statistical approaches to forcefield calibration and prediction uncertainty in molecular simulation. <i>Journal of Chemical Physics</i> , 2011 , 134, 054124	3.9	64
634	Rapid calculation of partition functions and free energies of fluids. <i>Journal of Chemical Physics</i> , 2011 , 135, 174105	3.9	24
633	Boiling point determination using adiabatic Gibbs ensemble Monte Carlo simulations: application to metals described by embedded-atom potentials. <i>Journal of Chemical Physics</i> , 2011 , 135, 224113	3.9	8
632	Needs and Opportunities -Molecular Modeling Meets Polymer Process Modeling. 2011 , 302, 6-15		3
631	Phase diagram of water under an applied electric field. 2011 , 107, 155702		41
630	A thermodynamic scaling Monte Carlo method to determine the unlike pair interaction parameter. 2011 ,		
629	Molecular simulation of swelling and structure for Na-Wyoming montmorillonite in supercritical CO ₂ . 2011 , 37, 1063-1070		18

628	Re-examining the properties of the aqueous vapor-liquid interface using dispersion corrected density functional theory. <i>Journal of Chemical Physics</i> , 2011 , 135, 124712	3.9	74
627	First principles predictions of thermophysical properties of refrigerant mixtures. <i>Journal of Chemical Physics</i> , 2011 , 134, 114518	3.9	5
626	Formation and structure of Al-Zr metallic glasses studied by Monte Carlo simulations. <i>Journal of Applied Physics</i> , 2011 , 109, 113538	2.5	35
625	Molecular dynamics simulations of vapor/liquid coexistence using the nonpolarizable water models. <i>Journal of Chemical Physics</i> , 2011 , 134, 124708	3.9	50
624	Chemical potential perturbation: a method to predict chemical potentials in periodic molecular simulations. <i>Journal of Chemical Physics</i> , 2011 , 134, 114514	3.9	10
623	Phase transitions of two-dimensional dipolar fluids in external fields. <i>Journal of Chemical Physics</i> , 2011 , 134, 114903	3.9	14
622	Simulation and theory of a model for tetrahedral colloidal particles. <i>Journal of Chemical Physics</i> , 2011 , 134, 194502	3.9	19
621	Communication: A simple method for simulation of freezing transitions. <i>Journal of Chemical Physics</i> , 2011 , 134, 171104	3.9	12
620	Vapor-liquid nucleation in two dimensions: on the intriguing sign switch of the errors of the classical nucleation theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 194304	3.9	6
619	SAFT-Force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models of n-decylbenzene. <i>Molecular Physics</i> , 2012 , 110, 1189-1203	1.7	71
618	Properties of patchy colloidal particles close to a surface: a Monte Carlo and density functional study. <i>Journal of Chemical Physics</i> , 2012 , 137, 084704	3.9	26
617	Phase behavior of colloids and proteins in aqueous suspensions: theory and computer simulations. <i>Journal of Chemical Physics</i> , 2012 , 137, 084905	3.9	64
616	Effective interactions in lysozyme aqueous solutions: a small-angle neutron scattering and computer simulation study. <i>Journal of Chemical Physics</i> , 2012 , 136, 035103	3.9	29
615	Inhomogeneous 2D Lennard-Jones Fluid: Theory and Computer Simulation. 2012 , 58, 759-764		3
614	Rejection-free Monte Carlo scheme for anisotropic particles. <i>Journal of Chemical Physics</i> , 2012 , 136, 144111	3.9	9
613	Mean Force Simulation of the Adsorption of Aqueous Dilute Solutions. 2012 , 10, 153-178		1
612	Demixing and field-induced population inversion in a mixture of neutral and dipolar-hard spheres confined in a slit pore. <i>Molecular Physics</i> , 2012 , 110, 1161-1169	1.7	5
611	Basic Concepts in Molecular Modeling. 2012 , 1-26		

610	Phase diagram of the modified Lennard-Jones system. <i>Journal of Chemical Physics</i> , 2012 , 137, 174502	3.9	25
609	Transferable potentials for phase equilibria-united atom description of five- and six-membered cyclic alkanes and ethers. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 11234-46	3.4	79
608	A systematic approach for development of an OPLS-like force field and its application to hydrofluorocarbons. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 14389-97	3.4	14
607	Molecular modeling of fluoropropene refrigerants. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 5744-51	3.4	49
606	Wang-Landau configurational bias Monte Carlo simulations: vapour-liquid equilibria of alkenes. 2012 , 38, 653-658		20
605	Simulation of phase boundaries using constrained cell models. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 375105	1.8	5
604	AZEOTROPE PREDICTION BY MONTE CARLO MOLECULAR SIMULATION. 2012 , 199, 673-688		1
603	Temperature- and pressure-dependent densities, self-diffusion coefficients, and phase behavior of monoacid saturated triacylglycerides: toward molecular-level insights into processing. 2012 , 60, 5243-9		15
602	Crowding-induced phase separation of Lennard-Jones particles: implications to nuclear structures in a biological cell. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 3874-9	3.4	12
601	Prediction of the PC-SAFT associating parameters by molecular simulation. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 367-77	3.4	26
600	Toward Quantitative Coarse-Grained Models of Lipids with Fluids Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1393-408	6.4	14
599	Transferable force field for carboxylate esters: application to fatty acid methyl ester phase equilibria prediction. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 3239-48	3.4	27
598	Molecular simulation of the phase behavior of fluids and fluid mixtures using the synthetic method. <i>Journal of Chemical Physics</i> , 2012 , 137, 054507	3.9	3
597	Monte Carlo simulations to study the forming ability and atomic configuration of the Cu-Al amorphous alloys. 2012 , 25, 109-114		5
596	Numerical estimate for boiling points via Wang-Landau simulations. 2012 , 38, 1265-1270		17
595	Incorporating configurational-bias Monte Carlo into the Wang-Landau algorithm for continuous molecular systems. <i>Journal of Chemical Physics</i> , 2012 , 137, 204105	3.9	4
594	Multicomponent adsorption of alcohols onto silicalite-1 from aqueous solution: isotherms, structural analysis, and assessment of ideal adsorbed solution theory. 2012 , 28, 15566-76		61
593	Constructing Molecular Models and Sampling Equilibrium Probability Distributions. 2012 , 191-226		1

592	Phase diagram of a two-dimensional system with anomalous liquid properties. <i>Journal of Chemical Physics</i> , 2012 , 137, 034507	3.9	26
591	Multiscale Molecular Methods in Applied Chemistry. 2012 ,		33
590	Computer simulations of nematic drops: coupling between drop shape and nematic order. <i>Journal of Chemical Physics</i> , 2012 , 137, 034505	3.9	15
589	Critical behaviour and vapour-liquid coexistence of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquids via Monte Carlo simulations. 2012 , 154, 53-69; discussion 81-96, 465-71		50
588	The influence of carbon dioxide cosolvent on solubility in poly(ethylene glycol). 2012 , 131, 1		4
587	Process Systems Engineering, 9. Domain Engineering. 2012 ,		
586	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. I. Thermodynamic properties in the bulk and at the liquid-vapor phase boundary. <i>Journal of Chemical Physics</i> , 2012 , 136, 184107	3.9	43
585	Modeling the Pressure Dependence of Acid Gas + n-Alkane Interfacial Tensions Using Atomistic Monte Carlo Simulations.. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 10563-10572	3.8	30
584	Phase diagram and universality of the Lennard-Jones gas-liquid system. <i>Journal of Chemical Physics</i> , 2012 , 136, 204102	3.9	83
583	Generalized approach to global renormalization-group theory for fluids. 2012 , 85, 041108		6
582	Determination of the solid-fluid coexistence of the n - 6 Lennard-Jones system from free energy calculations. <i>Journal of Chemical Physics</i> , 2012 , 136, 174502	3.9	28
581	Phase diagram of trivalent and pentavalent patchy particles. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 064113	1.8	22
580	Prediction of the mutual solubility of water and dipropylene glycol dimethyl ether using molecular dynamics simulation. <i>Fluid Phase Equilibria</i> , 2012 , 314, 1-6	2.5	8
579	Equilibrium and transport properties of CO ₂ + N ₂ O and CO ₂ + NO mixtures: Molecular simulation and equation of state modelling study. <i>Fluid Phase Equilibria</i> , 2012 , 322-323, 66-78	2.5	23
578	Prediction of critical properties for Naphthacene, Triphenylene and Chrysene by Wang-Landau simulations. <i>Fluid Phase Equilibria</i> , 2012 , 322-323, 92-96	2.5	18
577	A new and effective Bin-Monte Carlo scheme to study vapour-liquid equilibria and vapour-solid equilibria. <i>Fluid Phase Equilibria</i> , 2012 , 325, 53-65	2.5	12
576	Heating and sorption effects on silicalite-1 unit cell size and geometry. 2012 , 155, 65-70		7
575	Phase diagram of aluminum from EAM potentials. <i>European Physical Journal B</i> , 2013 , 86, 1	1.2	2

574	Calculation of the Gibbs free energy of solvation and dissociation of HCl in water via Monte Carlo simulations and continuum solvation models. 2013 , 15, 13578-85		31
573	GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium. 2013 , 184, 2662-2669		20
572	Selective adsorption from dilute solutions: Gibbs ensemble Monte Carlo simulations. <i>Fluid Phase Equilibria</i> , 2013 , 351, 1-6	2.5	9
571	Temperature-sensitive colloidal phase behavior induced by critical Casimir forces. <i>Journal of Chemical Physics</i> , 2013 , 139, 094903	3.9	38
570	TraPPE-zeo: Transferable Potentials for Phase Equilibria Force Field for All-Silica Zeolites. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 24375-24387	3.8	87
569	On the inner workings of Monte Carlo codes. 2013 , 39, 1253-1292		238
568	Influence of simulation protocols on the efficiency of Gibbs ensemble Monte Carlo simulations. 2013 , 39, 1135-1142		36
567	Statistical Mechanics. 2013 , 13-59		5
566	Overview of MedeA [®] -GIBBS capabilities for thermodynamic property calculation and VLE behaviour description of pure compounds and mixtures: application to polar compounds generated from ligno-cellulosic biomass. 2013 , 39, 1165-1211		14
565	Simulations of vapor-liquid phase equilibrium and interfacial tension in the CO ₂ -H ₂ O-NaCl system. 2013 , 59, 3514-3522		35
564	Molecular insights for the optimization of solvent-based selective extraction of ethanol from fermentation broths. 2013 , 59, 3065-3070		13
563	MCCCS Towhee: a tool for Monte Carlo molecular simulation. 2013 , 39, 1212-1222		189
562	The composition of ternary N ₂ /CH ₄ /C ₂ H ₆ cloud droplets under Titan conditions: Monte Carlo simulations and experiment. <i>Molecular Physics</i> , 2013 , 111, 2233-2242	1.7	1
561	A simplified representation of anisotropic charge distributions within proteins. <i>Journal of Chemical Physics</i> , 2013 , 138, 174110	3.9	11
560	Numerical self-consistent field theory of multicomponent polymer blends in the Gibbs ensemble. 2013 , 9, 11288		12
559	Vapour-liquid equilibrium (VLE) for the systems furan+n-hexane and furan+toluene. Measurements, data treatment and modeling using molecular models. <i>Fluid Phase Equilibria</i> , 2013 , 337, 234-245	2.5	20
558	Automated development of force fields for the calculation of thermodynamic properties: acetonitrile as a case study. 2013 , 39, 109-118		16
557	Molecular simulation studies of reversed-phase liquid chromatography. 2013 , 1287, 60-82		77

556	Solute extraction via supercritical ethane from poly(ethylene glycol): A Monte Carlo simulation study. <i>Fluid Phase Equilibria</i> , 2013 , 360, 351-356	2.5	2
555	Exploring fluctuations and phase equilibria in fluid mixtures via Monte Carlo simulation. 2013 , 34, 475-487		3
554	Sorption-induced structural transition of zeolitic imidazolate framework-8: a hybrid molecular simulation study. 2013 , 135, 3722-8		120
553	The influence of the liquid slab thickness on the planar vapor-liquid interfacial tension. 2013 , 392, 2359-2367		58
552	Use of the Grand Canonical Transition-Matrix Monte Carlo Method to Model Gas Adsorption in Porous Materials. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5861-5872	3.8	28
551	Simulating adsorptive expansion of zeolites: application to biomass-derived solutions in contact with silicalite. 2013 , 29, 4866-76		13
550	Monte Carlo simulations of water solubility and structures in poly(difluoromethylene). 2013 , 39, 367-384		1
549	Liquid-vapor equilibrium and interfacial properties of square wells in two dimensions. <i>Journal of Chemical Physics</i> , 2013 , 138, 044508	3.9	16
548	Mapping the phase diagram for neon to a quantum Lennard-Jones fluid using Gibbs ensemble simulations. <i>Journal of Chemical Physics</i> , 2013 , 138, 134502	3.9	11
547	Adsorption, intrusion and freezing in porous silica: the view from the nanoscale. 2013 , 42, 4141-71		171
546	Molecular Simulation Studies on the Vapor-Liquid Phase Equilibria of Binary Mixtures of R-1234yf and R-1234ze(E) with R-32 and CO ₂ . 2013 , 58, 1867-1873		68
545	Monte Carlo Simulation Methods for Computing Liquid-Vapor Saturation Properties of Model Systems. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2552-66	6.4	74
544	Intermolecular interactions and the thermodynamic properties of supercritical fluids. <i>Journal of Chemical Physics</i> , 2013 , 138, 194502	3.9	23
543	Vapor-liquid coexistence of the Stockmayer fluid in nonuniform external fields. 2013 , 87, 052128		6
542	Prediction of phase equilibrium and hydration free energy of carboxylic acids by Monte Carlo simulations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 7123-32	3.4	9
541	Grand canonical Monte Carlo simulations of vapor-liquid equilibria using a bias potential from an analytic equation of state. <i>Journal of Chemical Physics</i> , 2013 , 138, 234106	3.9	7
540	Phase-coexistence simulations of fluid mixtures by the Markov Chain Monte Carlo method using single-particle models. 2013 , 249, 233-248		1
539	Molecular Simulation Studies on the Thermophysical Properties of the Refrigerant Blend R-445A. 2013 , 58, 3470-3476		20

538	Efficient Combination of Environment Change and Alchemical Perturbation within the Enveloping Distribution Sampling (EDS) Scheme: Twin-System EDS and Application to the Determination of Octanol-Water Partition Coefficients. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1334-46	6.4	14
537	Transferable potentials for phase equilibria. 10. Explicit-hydrogen description of substituted benzenes and polycyclic aromatic compounds. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 273-88	3.4	77
536	Sublimation of the Modified Lennard-Jones System. 2013 , 82, 033001		5
535	Phase diagrams of Janus fluids with up-down constrained orientations. <i>Journal of Chemical Physics</i> , 2013 , 139, 174902	3.9	14
534	Chemical and topological short-range orders in the ternary Ni-Zr-Al metallic glasses studied by Monte Carlo simulations. <i>Journal of Physics Condensed Matter</i> , 2013 , 25, 095005	1.8	6
533	A comparative study of critical temperature estimation of atomic fluid and chain molecules using fourth-order Binder cumulant and simplified scaling laws. 2013 , 39, 154-159		7
532	Temperature measurement from perturbations. 2013 , 87,		5
531	Crystallization of asymmetric patchy models for globular proteins in solution. 2013 , 88, 012721		48
530	Monte Carlo simulation of the nonadditive restricted primitive model of ionic fluids: phase diagram and clustering. 2013 , 87, 052303		13
529	Computer simulation of liquid-vapor coexistence of confined quantum fluids. <i>Journal of Chemical Physics</i> , 2013 , 139, 184505	3.9	13
528	Acid Gases in CO ₂ -rich Subsurface Geologic Environments. 2013 , 77, 361-398		10
527	Prediction of Glass-Forming Ability and Atomic-Level Structure of the Al ₇₀ Zr ₃₀ Metallic Glasses by Molecular Dynamics Simulations. 2013 , 82, 124006		1
526	Fluid-solid equilibrium of carbon dioxide as obtained from computer simulations of several popular potential models: the role of the quadrupole. <i>Journal of Chemical Physics</i> , 2013 , 138, 084506	3.9	16
525	Cutoff Effect in the Nosé-Hoover and Nosé-Hoover Thermostats. 2013 , 82, 034001		2
524	Application of Gibbs Ensemble Monte Carlo to Phase Equilibria of CO ₂ /Hydrocarbon Mixtures. 2013 , ,		
523	Liquid-vapor equilibrium and surface properties of short rigid chains with one long range attractive potential. <i>Journal of Chemical Physics</i> , 2013 , 139, 024505	3.9	4
522	Isotherms of Fluids in Native and Defective Zeolite and Alumino-Phosphate Crystals: Monte-Carlo Simulations with On-the-Fly ab initio Electrostatic Potential. 2013 , 68, 299-307		2
521	10. Acid Gases in CO ₂ -rich Subsurface Geologic Environments. 2013 , 361-398		2

520	Equilibrium and Transport Properties of Primary, Secondary and Tertiary Amines by Molecular Simulation. 2014 , 69, 833-849		6
519	Simulating Phase Equilibria using Wang-Landau-Transition Matrix Monte Carlo. 2014 , 487, 012002		9
518	Theoretical and computer simulation study of phase coexistence of nonadditive hard-disk mixtures. <i>Journal of Chemical Physics</i> , 2014 , 141, 214508	3.9	6
517	Quantum Gibbs ensemble Monte Carlo. <i>Journal of Chemical Physics</i> , 2014 , 141, 114110	3.9	6
516	A Gibbs-ensemble based technique for Monte Carlo simulation of electric double layer capacitors (EDLC) at constant voltage. <i>Journal of Chemical Physics</i> , 2014 , 140, 174110	3.9	10
515	Twofold reentrant melting in a double-Gaussian fluid. <i>Journal of Chemical Physics</i> , 2014 , 140, 084906	3.9	8
514	Influence of system size on the properties of a fluid adsorbed in a nanopore: Physical manifestations and methodological consequences. <i>Journal of Chemical Physics</i> , 2014 , 141, 044716	3.9	5
513	Gibbs ensemble Monte Carlo of nonadditive hard-sphere mixtures. <i>Journal of Chemical Physics</i> , 2014 , 141, 044508	3.9	15
512	Phase behavior of a fluid with a double Gaussian potential displaying waterlike features. 2014 , 90, 012305		7
511	Gas-liquid coexistence for the boson square-well fluid and the (4)He binodal anomaly. 2014 , 90, 020102		4
510	Mapping coexistence lines via free-energy extrapolation: application to order-disorder phase transitions of hard-core mixtures. <i>Journal of Chemical Physics</i> , 2014 , 140, 094102	3.9	16
509	Quantifying Computational Effort Required for Stochastic Averages. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5229-34	6.4	21
508	Molecular simulation of thermodynamic and transport properties for the H ₂ O+NaCl system. <i>Journal of Chemical Physics</i> , 2014 , 141, 234507	3.9	49
507	Statistical scheduling of economic dispatch and energy reserves of hybrid power systems with high renewable energy penetration. 2014 ,		10
506	Crowding in polymer-nanoparticle mixtures. 2014 , 307, 27-71		26
505	Frontiers of stable isotope geoscience. 2014 , 372, 119-143		76
504	Assessing the ability of force-fields to predict liquid-liquid equilibria of ternary systems of light alcohols+water+dodecane by Monte Carlo simulation. <i>Fluid Phase Equilibria</i> , 2014 , 368, 65-71	2.5	7
503	Prediction of perfluorohexane adsorption in BCR-704 zeolite via molecular simulation. <i>Fluid Phase Equilibria</i> , 2014 , 366, 152-158	2.5	6

502	A computational study of the suppression of ammonia volatility in aqueous systems using ionic additives. 2014 , 25, 159-168		5
501	Molecular dynamics simulation of liquid-vapor phase diagrams of metals modeled using modified empirical pair potentials. <i>Fluid Phase Equilibria</i> , 2014 , 361, 181-187	2.5	5
500	Molecular Simulation of Ionic Liquids: Where We Are and the Path Forward. 2014 , 149-192		4
499	Long-range correction for multi-site Lennard-Jones models and planar interfaces. <i>Molecular Physics</i> , 2014 , 112, 2227-2234	1.7	19
498	A conservative and a hybrid early rejection schemes for accelerating Monte Carlo molecular simulation. <i>Molecular Physics</i> , 2014 , 112, 2575-2586	1.7	7
497	Fluid phase behavior of ethylene glycol+water mixtures (at operating conditions of the first-stage esterification reactors for PET synthesis) by molecular simulations and activity coefficient (γ) method. 2014 , 199, 565-571		3
496	Characterizing protein crystal contacts and their role in crystallization: rubredoxin as a case study. 2014 , 10, 290-302		43
495	Kinetic effects in predicting adsorption using the GCMC method Using CO ₂ adsorption on ZIFs as an example. 2014 , 4, 27571-27581		8
494	On the phase and interface behavior along the three-phase line of ternary Lennard-Jones mixtures: a collaborative approach based on square gradient theory and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2014 , 141, 014503	3.9	14
493	Prediction of Vapor-Liquid Coexistence Data for p-Cymene Using Equation of State Methods and Monte Carlo Simulations. 2014 , 59, 2987-2994		4
492	Monte Carlo simulations of phase behavior and microscopic structure for supercritical CO ₂ and thiophene mixtures. 2014 , 95, 214-221		5
491	Molecular Monte Carlo Simulation Method of Systems Connected to Three Reservoirs. 2014 , 83, 054003		
490	Competition between monomeric and dimeric crystals in schematic models for globular proteins. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 8034-41	3.4	9
489	Manifold Correction Method for the Nosé-Hoover and Nosé-Poincaré Molecular Dynamics Simulations. 2014 , 83, 024003		3
488	Prediction of Vapor-Liquid Coexistence Properties and Critical Points of Polychlorinated Biphenyls from Monte Carlo Simulations with the TraPPE-H Force Field. 2014 , 59, 3301-3306		7
487	Phase Coexistence Calculations of Reversibly Bonded Block Copolymers: A Unit Cell Gibbs Ensemble Approach. 2014 , 47, 1865-1874		10
486	Optimization of intermolecular potential parameters for the CO ₂ /H ₂ O mixture. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 11504-11	3.4	27
485	Impact of Associated Gases on Equilibrium and Transport Properties of a (CO_2) Stream: Molecular Simulation and Experimental Studies. 2014 , 35, 256-276		7

- 484 A computational study of the adsorption of n-perfluorohexane in zeolite BCR-704. *Fluid Phase Equilibria*, **2014**, 366, 146-151 2.5 13
- 483 Vapor-liquid equilibrium simulation of binary and ternary mixtures of CH₄, C₂H₄ and iso-C₄H₁₀. **2014**, 20, 79-85
- 482 Deconstructing Hydrogen-Bond Networks in Confined Nanoporous Materials: Implications for Alcohol/Water Separation. *Journal of Physical Chemistry C*, **2014**, 118, 19723-19732 3.8 40
- 481 Mie Potentials for Phase Equilibria: Application to Alkenes. **2014**, 59, 3144-3150 24
- 480 Predicting adsorption of n-perfluorohexane in BCR-704 by molecular simulation. *Fluid Phase Equilibria*, **2014**, 366, 165-170 2.5 4
- 479 High-pressure interfacial tensions for nitrogen+ethanol, or hexane or 2-methoxy-2-methylbutane: A comparison between experimental tensiometry and Monte Carlo simulations. **2014**, 89, 78-88 23
- 478 Molecular-level simulation of bubble and dew points of fluid mixtures and application to refrigerant cycle design. **2014**, 42, 1-7 5
- 477 Equilibrium and non-equilibrium cluster phases in colloids with competing interactions. **2014**, 10, 4479-86 50
- 476 Phase equilibria, fluid structure, and diffusivity of a discotic liquid crystal. **2014**, 10, 3171-82 15
- 475 Atomistic Simulations of Properties and Phenomena at High Temperatures. **2014**, 287-393 1
- 474 Hierarchical Modeling of Polymeric Systems at Multiple Time and Length Scales. **2014**, 85-134
- 473 On Stochastic Error and Computational Efficiency of the Markov Chain Monte Carlo Method. **2014**, 16, 467-490 1
- 472 Off-lattice models. 212-281
- 471 Two-phase coexistence for hydrogen-helium mixtures. **2015**, 92, 012133 3
- 470 Atomistic Design of Favored Compositions for Synthesizing the Al-Ni-Y Metallic Glasses. **2015**, 5, 16218 5
- 469 Reactivity and Dynamics at Liquid Interfaces. **2015**, 205-313 4
- 468 Computer Simulations of Biaxial Nematics. **2015**, 153-184 1
- 467 Accurate and precise determination of critical properties from Gibbs ensemble Monte Carlo simulations. *Journal of Chemical Physics*, **2015**, 143, 114113 3.9 38

466	Understanding the sensitivity of nucleation free energies: The role of supersaturation and temperature. <i>Journal of Chemical Physics</i> , 2015 , 143, 164516	3.9	5
465	Calculating phase equilibrium properties of plasma pseudopotential model using hybrid Gibbs statistical ensemble Monte-Carlo technique. 2015 , 653, 012124		1
464	. 2015 ,		44
463	Coarsening in fluid phase transitions. 2015 , 16, 303-315		12
462	Ab initio Intermolecular Potential Energy Surface and Calculation of Second Virial Coefficients for the Cl ₂ -Cl ₂ Dimer. 2015 , 3, 193-201		6
461	Prediction of Surface and Bulk Partition of Nonionic Surfactants Using Free Energy Calculations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 15623-30	3.4	11
460	Etomica: an object-oriented framework for molecular simulation. 2015 , 36, 573-83		21
459	Adsorption of argon on graphite and graphite with preadsorbed xenon monolayer: Simulation using the Monte Carlo technique. 2015 , 51, 57-65		1
458	Recent advances in molecular simulation: A chemical engineering perspective. 2015 , 61, 370-383		44
457	Classical force field for hydrofluorocarbon molecular simulations. Application to the study of gas solubility in poly(vinylidene fluoride). 2015 , 119, 140-51		25
456	Vapor-liquid equilibria for the binary systems ethylene+water, ethylene+ethanol, and ethanol+water, and the ternary system ethylene+water+ethanol from Gibbs-ensemble molecular simulation. <i>Fluid Phase Equilibria</i> , 2015 , 394, 1-11	2.5	5
455	Effect of an external field on the structure and the phase transitions of a confined mixture of neutral and dipolar hard spheres. <i>Molecular Physics</i> , 2015 , 113, 3216-3227	1.7	2
454	Vapor-phase chemical equilibrium and combined chemical and vapor-liquid equilibrium for the ternary system ethylene + water + ethanol from reaction-ensemble and reactive Gibbs-ensemble molecular simulations. <i>Fluid Phase Equilibria</i> , 2015 , 403, 104-113	2.5	1
453	Improved Monte Carlo Scheme for Efficient Particle Transfer in Heterogeneous Systems in the Grand Canonical Ensemble: Application to Vapor-Liquid Nucleation. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4023-32	6.4	11
452	Surface tension of the two center Lennard-Jones plus quadrupole model fluid. <i>Fluid Phase Equilibria</i> , 2015 , 392, 12-18	2.5	12
451	Development of the Transferable Potentials for Phase Equilibria Model for Hydrogen Sulfide. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 7041-52	3.4	37
450	Thermodynamic predicting and atomistic modeling the favored compositions for Mg ₇₀ Ni ₃₀ metallic glasses. 2015 , 5, 60220-60229		3
449	Molecular Simulation Studies on the Vapor-liquid Equilibria of the cis- and trans-HCFO-1233zd and the cis- and trans-HFO-1336mzz. 2015 , 60, 2412-2419		36

448	Thermodynamic and Transport Properties of H ₂ O + NaCl from Polarizable Force Fields. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3802-10	6.4	49
447	Extension of the TraPPE-UA force field to the simulation of vapor-liquid phase equilibria of vinyl acetate system. 2015 , 209, 520-525		8
446	Constant pressure Gibbs ensemble Monte Carlo simulations for the prediction of structure I gas hydrate occupancy. 2015 , 26, 446-452		17
445	Ab Initio Derived Force Fields for Predicting CO ₂ Adsorption and Accessibility of Metal Sites in the Metal-Organic Frameworks M-MOF-74 (M = Mn, Co, Ni, Cu). <i>Journal of Physical Chemistry C</i> , 2015 , 119, 16058-16071	3.8	67
444	Brownian motion of a nano-colloidal particle: the role of the solvent. 2015 , 17, 19557-68		11
443	Effects of Critical Fluctuations on Adsorption-Induced Deformation of Microporous Carbons. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 6111-6120	3.8	8
442	A corresponding-states framework for the description of the Mie family of intermolecular potentials. <i>Molecular Physics</i> , 2015 , 113, 932-947	1.7	47
441	Vapor-liquid equilibria of CH ₄ , CO ₂ and their binary system CH ₄ + CO ₂ : A comparison between the molecular simulation and equation of state. 2015 , 58, 650-658		4
440	Improving Monte-Carlo and Molecular Dynamics Simulation Outcomes Using Temperature-Dependent Interaction Parameters: The Case of Pure LJ Fluid. 2015 , 12, 1550003		4
439	Monte Carlo simulation and SAFT modeling study of the solvation thermodynamics of dimethylformamide, dimethylsulfoxide, ethanol and 1-propanol in the ionic liquid trimethylbutylammonium bis(trifluoromethylsulfonyl)imide. 2015 , 17, 7449-62		9
438	Molecular modeling and simulation of vapor-liquid equilibrium of the refrigerant R152a and its mixture R152a+R32. <i>Fluid Phase Equilibria</i> , 2015 , 394, 93-100	2.5	9
437	Optimized Mie potentials for phase equilibria: Application to noble gases and their mixtures with n-alkanes. <i>Journal of Chemical Physics</i> , 2015 , 143, 114504	3.9	33
436	Water Sites, Networks, And Free Energies with Grand Canonical Monte Carlo. 2015 , 137, 14930-43		68
435	Monte Carlo Simulations Probing the Adsorptive Separation of Hydrogen Sulfide/Methane Mixtures Using All-Silica Zeolites. 2015 , 31, 12268-78		27
434	Isotropic-nematic phase equilibria of hard-sphere chain fluids-Pure components and binary mixtures. <i>Journal of Chemical Physics</i> , 2015 , 142, 064903	3.9	7
433	Extended law of corresponding states for protein solutions. <i>Journal of Chemical Physics</i> , 2015 , 142, 174995	3.5	45
432	Transferable Anisotropic United-Atom Force Field Based on the Mie Potential for Phase Equilibrium Calculations: n-Alkanes and n-Olefins. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11695-707	3.4	38
431	Liquid-liquid equilibria for soft-repulsive particles: improved equation of state and methodology for representing molecules of different sizes and chemistry in dissipative particle dynamics. <i>Journal of Chemical Physics</i> , 2015 , 142, 044902	3.9	19

430	Optimizing Noble Gas-Water Interactions via Monte Carlo Simulations. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 14486-95	3-4	11
429	Solubility of Carbon Dioxide in Pentaerythritol Hexanoate: Molecular Dynamics Simulation of a Refrigerant-Lubricant Oil System. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 12274-80	3-4	5
428	Gibbs ensemble Monte Carlo. 2015 , 83, 809-816		4
427	Hydrothermal properties of the COS/D2 water model: a polarizable charge-on-spring water model, at elevated temperatures and pressures. 2015 , 5, 75846-75856		1
426	Transferability and nonbond functional form of coarse grained force field - tested on linear alkanes. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4760-9	6-4	30
425	An analytical equation of state for describing isotropic-nematic phase equilibria of Lennard-Jones chain fluids with variable degree of molecular flexibility. <i>Journal of Chemical Physics</i> , 2015 , 142, 244903	3-9	11
424	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. 2015 , 115, 13093-164		87
423	Phase behavior of electrostatically complexed polyelectrolyte gels using an embedded fluctuation model. 2015 , 11, 1214-25		47
422	A Monte Carlo Simulation Study To Predict the Solubility of Carbon Dioxide, Hydrogen, and Their Mixture in the Ionic Liquids 1-Alkyl-3-methylimidazolium bis(trifluoromethanesulfonyl)amide ([Cnmim+][Tf2N] n = 4, 6). <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 4385-4395	3-9	18
421	Triple point of Belf Coulomb plasma model calculated using hybrid Gibbs ensemble technique. 2016 , 774, 012158		
420	Modeling Mechanism and Growth Reactions for New Nanofabrication Processes by Atomic Layer Deposition. 2016 , 28, 5367-80		48
419	Improving performance of GPU code using novel features of the NVIDIA kepler architecture. 2016 , 28, 3586-3605		5
418	Pore size tuning of poly(styrene-co-vinylbenzyl chloride-co-divinylbenzene) hypercrosslinked polymers: Insights from molecular simulations. 2016 , 99, 173-184		21
417	Single-site Lennard-Jones models via polynomial chaos surrogates of Monte Carlo molecular simulation. <i>Journal of Chemical Physics</i> , 2016 , 144, 214301	3-9	
416	High Charge Density Coacervate Assembly via Hybrid Monte Carlo Single Chain in Mean Field Theory. 2016 , 49, 9693-9705		30
415	Equation of State for the Lennard-Jones Fluid. 2016 , 45, 023101		97
414	Perspective: How good is DFT for water?. <i>Journal of Chemical Physics</i> , 2016 , 144, 130901	3-9	451
413	Molecular simulation of the thermodynamic, structural, and vapor-liquid equilibrium properties of neon. <i>Journal of Chemical Physics</i> , 2016 , 145, 104501	3-9	20

412	The second virial coefficient and critical point behavior of the Mie Potential. <i>Journal of Chemical Physics</i> , 2016 , 145, 084505	3.9	11
411	Evaluation of the grand-canonical partition function using expanded Wang-Landau simulations. IV. Performance of many-body force fields and tight-binding schemes for the fluid phases of silicon. <i>Journal of Chemical Physics</i> , 2016 , 144, 124510	3.9	20
410	Phase behavior of patchy spheroidal fluids. <i>Journal of Chemical Physics</i> , 2016 , 145, 214904	3.9	5
409	A new intermolecular potential for simulations of methanol: The OPLS/2016 model. <i>Journal of Chemical Physics</i> , 2016 , 145, 034508	3.9	22
408	Characterisation of the thermodynamics, structure and dynamics of a water-like model in 2- and 3-dimensions. 2016 , 18, 17335-40		9
407	Lessons learned from theory and simulation of step potentials. <i>Fluid Phase Equilibria</i> , 2016 , 416, 27-41	2.5	5
406	Test of athermal terms of activity coefficients by large scale molecular dynamics simulation for vapor-liquid equilibria. <i>Fluid Phase Equilibria</i> , 2016 , 420, 20-23	2.5	
405	Gate opening effect for carbon dioxide in ZIF-8 by molecular dynamics [Confirmed, but at high CO2 pressure. 2016 , 648, 178-181		29
404	A new insight to validation of local composition models in binary mixtures using molecular dynamic simulation. 2016 , 62, 275-286		4
403	Characterization of the structural collapse undergone by an unstable system of ultrasoft particles. 2016 , 457, 492-505		5
402	Optimization of Particle Transfers in the Gibbs Ensemble for Systems with Strong and Directional Interactions Using CBMC, CFCMC, and CB/CFCMC. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 9148-9159	3.8	15
401	Molecular Simulation of Olefin Oligomer Blend Phase Behavior. 2016 , 49, 3975-3985		17
400	CO2 Adsorption in M-IRMOF-10 (M = Mg, Ca, Fe, Cu, Zn, Ge, Sr, Cd, Sn, Ba). <i>Journal of Physical Chemistry C</i> , 2016 , 120, 12819-12830	3.8	18
399	Molecular simulation studies in hydrofluoroolefine (HFO) working fluids and their blends. 2016 , 22, 1077-1089		24
398	Binary Lennard-Jones mixtures with highly asymmetric interactions of the components. 1. Effect of the energy parameters on phase equilibria and properties of liquid-gas interfaces. <i>Fluid Phase Equilibria</i> , 2016 , 429, 242-253	2.5	15
397	Effect of confinement in nano-porous materials on the solubility of a supercritical gas. <i>Molecular Physics</i> , 2016 , 114, 3294-3306	1.7	23
396	Predictive evaluation of phase equilibria in biofuel systems using molecular thermodynamic models. 2016 , 118, 64-78		8
395	Pathways to self-organization: Crystallization via nucleation and growth. 2016 , 39, 77		29

- 394 A new optimization method for the determination of classical force fields. Application to the united atom force field of short alkanes. *Fluid Phase Equilibria*, **2016**, 429, 27-36 2.5 3
- 393 Monte Carlo Simulation of Near- and Supercritical Hexane Fluid and Physisorption Phase Behavior. *Journal of Physical Chemistry C*, **2016**, 120, 21336-21343 3.8
- 392 Molecular Simulation of Polymer Melts and Blends: Methods, Phase Behavior, Interfaces, and Surfaces. **2016**, 1-44
- 391 Binary Lennard-Jones mixtures with highly asymmetric interactions of the components. 2. Effect of the particle size on phase equilibria and properties of liquid-gas interfaces. *Fluid Phase Equilibria*, **2016**, 430, 67-74 2.5 10
- 390 Determining pressure-temperature phase diagrams of materials. **2016**, 93, 31
- 389 Recent Developments in Fully Fluctuating Field-Theoretic Simulations of Polymer Melts and Solutions. *Journal of Physical Chemistry B*, **2016**, 120, 7615-34 3.4 71
- 388 Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water. *Journal of Physical Chemistry B*, **2016**, 120, 12358-12370 3.4 28
- 387 Phase behavior of a binary fluid mixture of quadrupolar molecules. **2016**, 94, 052601 3
- 386 Statistical Surface Thermodynamics. **2016**, 883-1253 5
- 385 Leveraging Gibbs Ensemble Molecular Dynamics and Hybrid Monte Carlo/Molecular Dynamics for Efficient Study of Phase Equilibria. *Journal of Chemical Theory and Computation*, **2016**, 12, 5501-5510 6.4 6
- 384 Reverse energy partitioning-An efficient algorithm for computing the density of states, partition functions, and free energy of solids. *Journal of Chemical Physics*, **2016**, 145, 084116 3.9 4
- 383 Atomistic Modeling and Simulation for Solving Gas Extraction Problems. **2016**, 137-151 3
- 382 Predicting the adsorption of n-perfluorohexane (n-C₆F₁₄) on BAM-P109 activated carbon using an ab initio force field. **2016**, 34, 110-122 1
- 381 Gibbs ensemble Monte Carlo simulation using an optimized potential model: pure acetic acid and a mixture of it with ethylene. **2016**, 22, 162 6
- 380 Scaling Laws and Critical Properties for fcc and hcp Metals. *Journal of Physical Chemistry B*, **2016**, 120, 5255-61 3.4 20
- 379 Foundations of Molecular Modeling and Simulation. **2016**,
- 378 Vapor Liquid Equilibria of Hydrofluorocarbons Using Dispersion-Corrected and Nonlocal Density Functionals. *Journal of Chemical Theory and Computation*, **2016**, 12, 3295-304 6.4 9
- 377 Vapor-liquid phase equilibrium diagram for uranium hexafluoride (UF₆) using simplified temperature dependent intermolecular potential parameters (TDIP). **2016**, 310, 139-154 2

376	Monte Carlo simulations of H ₂ O/NaCl ₂ and H ₂ O/NaCl ₂ /CO ₂ mixtures. <i>Fluid Phase Equilibria</i> , 2016 , 407, 262-268	2.5	11
375	Modeling and Simulation Environments for Sustainable Low-Carbon Energy Production [A Review]. 2016 , 11, 97-124		6
374	Molecular simulations of supercritical fluid systems. 2016 , 108, 104-122		42
373	Molecular simulation of ethylene-expanded methanol: Phase behavior, structure, and transport properties. <i>Fluid Phase Equilibria</i> , 2016 , 411, 81-87	2.5	6
372	Adsorptive Separation of 1-Butanol from Aqueous Solutions Using MFI- and FER-Type Zeolite Frameworks: A Monte Carlo Study. 2016 , 32, 2093-101		24
371	Gaussian-Charge Polarizable and Nonpolarizable Models for CO ₂ . <i>Journal of Physical Chemistry B</i> , 2016 , 120, 984-94	3.4	25
370	Direct Free Energy Calculation in the Continuous Fractional Component Gibbs Ensemble. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1481-90	6.4	35
369	Critical Casimir forces for colloidal assembly. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 043001	1.8	15
368	Computer modelling of the surface tension of the gas-liquid and liquid-liquid interface. 2016 , 45, 1387-409		121
367	Exact matrix treatment of an osmotic ensemble model of adsorption and pressure induced structural transitions in metal organic frameworks. 2016 , 45, 4213-7		13
366	Stability of the kaolinite-guest molecule intercalation system: A molecular simulation study. <i>Fluid Phase Equilibria</i> , 2016 , 409, 434-438	2.5	4
365	A Monte Carlo simulation study of the liquid-liquid equilibria for binary dodecane/ethanol and ternary dodecane/ethanol/water mixtures. <i>Fluid Phase Equilibria</i> , 2016 , 407, 269-279	2.5	22
364	Monte Carlo simulations of water solubility in ionic liquids: A force field assessment. <i>Fluid Phase Equilibria</i> , 2016 , 407, 117-125	2.5	25
363	Speeding up Monte Carlo molecular simulation by a non-conservative early rejection scheme. 2016 , 42, 229-241		2
362	Osmosis and thermodynamics explained by solute blocking. 2017 , 46, 59-64		5
361	Phase Equilibria of Water/CO and Water/n-Alkane Mixtures from Polarizable Models. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 1386-1395	3.4	21
360	Droplet growth during vapor-liquid transition in a 2D Lennard-Jones fluid. <i>Journal of Chemical Physics</i> , 2017 , 146, 024503	3.9	6
359	Applications of molecular simulations for separation and adsorption in zeolites. 2017 , 242, 294-348		44

358	Multi-Cell Monte Carlo Relaxation method for predicting phase stability of alloys. 2017 , 132, 9-12		20
357	Assessment and Optimization of Configurational-Bias Monte Carlo Particle Swap Strategies for Simulations of Water in the Gibbs Ensemble. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 431-440	6.4	18
356	Monte Carlo predictions for vapor-liquid equilibria of N-Methyl-2-pyrrolidone + benzene + thiophene. 2017 , 230, 28-35		1
355	Blocking effect of benzene-like fluid transport in nanoscale block-pores. 2017 , 43, 526-533		5
354	Phase behaviour in complementary DNA-coated gold nanoparticles and fd-viruses mixtures: a numerical study. 2017 , 40, 7		3
353	Estimating the solubility of 1:1 electrolyte aqueous solutions: the chemical potential difference rule. <i>Molecular Physics</i> , 2017 , 115, 1301-1308	1.7	14
352	Finite-size scaling study of dynamic critical phenomena in a vapor-liquid transition. <i>Journal of Chemical Physics</i> , 2017 , 146, 044503	3.9	8
351	Calculation of second virial coefficients using ab initio intermolecular pair potentials for F2-F2 and H2-F2 dimers. 2017 , 485-486, 67-80		8
350	Using the k-d Tree Data Structure to Accelerate Monte Carlo Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1556-1565	6.4	12
349	Accurate Critical Parameters for the Modified Lennard-Jones Model. 2017 , 86, 034003		2
348	Applying group functions to description of ionic liquids. 2017 , 1116, 141-150		3
347	Optimized Mie Potentials for Phase Equilibria: Application to Branched Alkanes. 2017 , 62, 1806-1818		17
346	Software Platforms for Electronic/Atomistic/Mesosopic Modeling: Status and Perspectives. 2017 , 6, 92-110		4
345	Theoretical study of carbon dioxide adsorption and diffusion in MIL-127(Fe) metal organic framework. 2017 , 491, 118-125		9
344	Computational Modeling and Simulation of CO Capture by Aqueous Amines. 2017 , 117, 9524-9593		86
343	Monte Carlo simulations of vapour-liquid phase equilibrium and microstructure for the system containing azeotropes. 2017 , 43, 1125-1133		4
342	Determining the critical points and coexistence curve of multi-species equilibria using Gaussian Process Regression. <i>Fluid Phase Equilibria</i> , 2017 , 449, 197-206	2.5	
341	Determination of the vapor-liquid transition of square-well particles using a novel generalized-canonical-ensemble-based method. 2017 , 26, 060202		2

340	Improved Solvents for CO ₂ Capture by Molecular Simulation Methodology. 2017 , 147-160		
339	Transferable potentials for phase equilibria. Improved united-atom description of ethane and ethylene. 2017 , 63, 5098-5110		20
338	Thermodynamic behavior of charged Lennard-Jones fluids. 2017 , 234, 424-429		7
337	Molecular Simulation Methods for CO ₂ Capture and Gas Separation with Emphasis on Ionic Liquids. 2017 , 79-111		2
336	Optimised Mie potentials for phase equilibria: application to alkynes. <i>Molecular Physics</i> , 2017 , 115, 1378-1388	10	
335	Computation of thermodynamic properties in the continuous fractional component Monte Carlo Gibbs ensemble. 2017 , 43, 189-195		17
334	Free Energy-Based Coarse-Grained Force Field for Binary Mixtures of Hydrocarbons, Nitrogen, Oxygen, and Carbon Dioxide. 2017 , 57, 50-59		14
333	Benchmark Free Energies and Entropies for Saturated and Compressed Water. 2017 , 62, 4032-4040		6
332	Deconstructing the Confinement Effect upon the Organization and Dynamics of Water in Hydrophobic Nanoporous Materials: Lessons Learned from Zeolites. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 22015-22024	3.8	21
331	Replica-Exchange and Standard State Binding Free Energies with Grand Canonical Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6373-6381	6.4	19
330	Metal-Nonmetal Transition in Fluid Cesium: A Many-Body Dissipative Particle Dynamics Simulation Approach. 2017 , 62, 3938-3945		2
329	NLDFT Pore Size Distribution in Amorphous Microporous Materials. 2017 , 33, 11138-11145		84
328	Pressure Enhancement in Confined Fluids: Effect of Molecular Shape and Fluid-Wall Interactions. 2017 , 33, 11231-11245		26
327	Simulating Osmotic Equilibria: A New Tool for Calculating Activity Coefficients in Concentrated Aqueous Salt Solutions. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 9647-9658	3.4	5
326	Experimental and theoretical investigations of the gas adsorption sites in rht-metal-organic frameworks. 2017 , 19, 4646-4665		14
325	Simultaneous Description of Equilibrium, Interfacial, and Transport Properties of Fluids Using a Mie Chain Coarse-Grained Force Field. <i>Industrial & Engineering Chemistry Research</i> , 2017 , 56, 9213-9226	3.9	35
324	Prediction of binary phase behavior for supercritical carbon dioxide + 1-pentanol, 2-pentanone, 1-octene or ethylbenzene via molecular simulation. 2017 , 245, 91-96		1
323	Molecular dynamics and Monte Carlo simulation of the structural properties, diffusion and adsorption of poly (amide-6-b-ethylene oxide)/Faujasite mixed matrix membranes. 2017 , 242, 404-415		11

322	Comparative Study of the Effect of Defects on Selective Adsorption of Butanol from Butanol/Water Binary Vapor Mixtures in Silicalite-1 Films. 2017 , 33, 8420-8427		19
321	Field-Theoretic Simulations of the Distribution of Nanorods in Diblock Copolymer Thin Films. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 11198-11209	3-4	8
320	Phase Behavior in Shale Organic and Inorganic Nanopores From Molecular Simulation. 2017 ,		1
319	Simulated molecular-scale interaction of supercritical fluid mobile and stationary phases. 2017 , 1527, 97-104		1
318	Self-intermediate scattering function analysis of supercooled water confined in hydrophilic silica nanopores. <i>Journal of Chemical Physics</i> , 2017 , 146, 214501	3-9	12
317	Influence of fluorination on barrier properties of polymers: Insights from Monte Carlo simulations of eicosanes + methane. 2017 , 40, 12		1
316	Predicting vapor-liquid phase equilibria with augmented ab initio interatomic potentials. <i>Journal of Chemical Physics</i> , 2017 , 146, 244504	3-9	11
315	Surface wettability effect on fluid transport in nanoscale slit pores. 2017 , 63, 1704-1714		33
314	A new kinetic Monte Carlo scheme with Gibbs ensemble to determine vapour-liquid equilibria. 2017 , 43, 76-85		8
313	Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations. <i>Fluid Phase Equilibria</i> , 2017 , 433, 50-55	2-5	26
312	Transferable Coarse-Grained Models of Liquid-Liquid Equilibrium Using Local Density Potentials Optimized with the Relative Entropy. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 5678-5693	3-4	36
311	Statistical mechanics of binary mixture adsorption in metal-organic frameworks in the osmotic ensemble. 2018 , 376,		10
310	Universal behavior of soft-core fluids near the threshold of thermodynamic stability. <i>Journal of Chemical Physics</i> , 2018 , 148, 084904	3-9	4
309	Many-body interactions between charged particles in a polymer solution: the protein regime. 2018 , 14, 4064-4073		2
308	Computational Design of High-Block Oligomers for Accessing 1 nm Domains. 2018 , 12, 4351-4361		18
307	Transferable Potentials for Chloroethenes: Insights into Nonideal Solution Behavior of Environmental Contaminants. <i>ACS Omega</i> , 2018 , 3, 3646-3654	3-9	1
306	Role of a reaction coordinate in free energy calculations. 2018 , 44, 1033-1043		1
305	Thermodynamic properties of confined square-well fluids with multiple associating sites. <i>Journal of Chemical Physics</i> , 2018 , 148, 074703	3-9	4

- 304 Pressure control in interfacial systems: Atomistic simulations of vapor nucleation. *Journal of Chemical Physics*, **2018**, 148, 064706 3.9 10
- 303 Molecular simulations of a CO₂/CO mixture in MIL-127. **2018**, 696, 86-91 7
- 302 Molecular simulations in drug delivery: Opportunities and challenges. **2018**, 8, e1358 32
- 301 A Novel Microemulsion Phase Transition: Toward the Elucidation of Third-Phase Formation in Spent Nuclear Fuel Reprocessing. *Journal of Physical Chemistry B*, **2018**, 122, 1439-1452 3.4 30
- 300 Solubility of CO₂ in triglycerides using Monte Carlo simulations. *Fluid Phase Equilibria*, **2018**, 476, 39-47 2.5 7
- 299 Grand canonical Monte Carlo and molecular dynamics simulations of the structural properties, diffusion and adsorption of hydrogen molecules through poly(benzimidazoles)/nanoparticle oxides composites. *International Journal of Hydrogen Energy*, **2018**, 43, 2803-2816 6.7 14
- 298 Force Field Benchmark of the TraPPE-UA for Polar Liquids: Density, Heat of Vaporization, Dielectric Constant, Surface Tension, Volumetric Expansion Coefficient, and Isothermal Compressibility. *Journal of Physical Chemistry B*, **2018**, 122, 1669-1678 3.4 15
- 297 Thermodynamic study of binary systems containing sulphur dioxide and nitric oxide: Measurements and modelling. *Fluid Phase Equilibria*, **2018**, 461, 84-100 2.5 3
- 296 Liquid-Liquid Phase Separation of Patchy Particles Illuminates Diverse Effects of Regulatory Components on Protein Droplet Formation. **2018**, 8, 6728 65
- 295 Calculation of excess free energy of molecular solids comprised of flexible molecules using Einstein molecule method. **2018**, 44, 781-788 5
- 294 Thermodynamic and transport properties of nitrogen fluid: Molecular theory and computer simulations. **2018**, 506, 36-44 3
- 293 Guaiacol and its mixtures: New data and predictive models part 1: Phase equilibrium. *Fluid Phase Equilibria*, **2018**, 470, 75-90 2.5 4
- 292 Ionic-Functionalized Polymers of Intrinsic Microporosity for Gas Separation Applications. **2018**, 34, 3949-3960 15
- 291 Reproducing Quantum Probability Distributions at the Speed of Classical Dynamics: A New Approach for Developing Force-Field Functors. **2018**, 9, 1721-1727 1
- 290 Molecular simulation of binary phase diagrams from the osmotic equilibrium method: vapour pressure and activity in water-ethanol mixtures. *Molecular Physics*, **2018**, 116, 2009-2021 1.7 6
- 289 A Monte Carlo simulation study of the interfacial tension for water/oil mixtures at elevated temperatures and pressures: Water/n-dodecane, water/toluene, and water/(n-dodecane + toluene). *Fluid Phase Equilibria*, **2018**, 476, 16-24 2.5 16
- 288 Critical temperature estimation of bulk and confined atomic fluid using vapour-liquid interfacial free energy. **2018**, 44, 156-163 1
- 287 An effective way to determine the melting curve. **2018**, 44, 384-388

286	Gibbs ensemble Monte Carlo simulations of multicomponent natural gas mixtures. 2018 , 44, 377-383		8
285	Performance of density functionals for modeling vapor liquid equilibria of CO and SO. 2018 , 39, 397-406		8
284	CO ₂ solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. <i>Fluid Phase Equilibria</i> , 2018 , 458, 1-8	2.5	7
283	Liquid-Vapor Phase Diagram of RPBE-D3 Water: Electronic Properties along the Coexistence Curve and in the Supercritical Phase. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 3318-3329	3.4	26
282	Absorption. 2018 , 1-115		0
281	Precise estimation of transfer free energies for ionic species between similar media. 2018 , 20, 27003-27010		0
280	Microscopic Origin of Frictional Rheology in Dense Suspensions: Correlations in Force Space. 2018 , 121, 128002		23
279	Dissipative particle dynamics modeling of hydrogel swelling by osmotic ensemble method. <i>Journal of Chemical Physics</i> , 2018 , 149, 094904	3.9	12
278	Insights into Noncovalent Binding Obtained from Molecular Dynamics Simulations. 2018 , 90, 1864-1875		8
277	A Hybrid Monte Carlo Self-Consistent Field Model of Physical Gels of Telechelic Polymers. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6532-6543	6.4	4
276	Monte Carlo Simulations of Fluid Phase Equilibria and Interfacial Properties for Water/Alkane Mixtures: An Assessment of Nonpolarizable Water Models and of Departures from the Lorentz-Berthelot Combining Rules. 2018 , 63, 4256-4268		12
275	Flat-Histogram Monte Carlo as an Efficient Tool To Evaluate Adsorption Processes Involving Rigid and Deformable Molecules. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6149-6158	6.4	10
274	Predicting the Features of Methane Adsorption in Large Pore Metal-Organic Frameworks for Energy Storage. 2018 , 8,		12
273	Integrated QMMM and Monte Carlo methods for analysis of adsorptive interactions between goethite cluster, carbon nanotubes, and arsenate. 2018 , 118, e25653		
272	Vapor-liquid equilibrium and equation of state of two-dimensional fluids from a discrete perturbation theory. <i>Journal of Chemical Physics</i> , 2018 , 148, 194505	3.9	6
271	A review of molecular simulation applied in vapor-liquid equilibria (VLE) estimation of thermodynamic cycles. 2018 , 264, 652-674		10
270	Intermolecular Potential-Based Equations of State from Molecular Simulation and Second Virial Coefficient Properties. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7757-7763	3.4	8
269	Phase Behavior in Shale Organic/Inorganic Nanopores From Molecular Simulation. 2018 , 21, 626-637		11

- 268 Understanding the unique sorption of alkane-, -diols in silicalite-1. *Journal of Chemical Physics*, **2018**, 149, 072331 3.9 5
- 267 A molecular simulation approach to the computation of mutual solubility of water and organic liquids: Application to fatty acids. *Fluid Phase Equilibria*, **2018**, 472, 48-55 2.5 6
- 266 Understanding the Molecular Weight Dependence of χ and the Effect of Dispersity on Polymer Blend Phase Diagrams. **2018**, 51, 3774-3787 13
- 265 Using molecular simulations to probe pore structures and polymer partitioning in size exclusion chromatography. **2018**, 1573, 78-86 7
- 264 Vapor-Liquid Equilibria of Mixtures of Molecular Fluids Using the Activity Fraction Expanded Ensemble Simulation Method. *Industrial & Engineering Chemistry Research*, **2018**, 57, 12235-12248 3.9 1
- 263 Programming configurational changes in systems of functionalised polymers using reversible intramolecular linkages. *Molecular Physics*, **2018**, 116, 2927-2941 1.7 4
- 262 Statistical fluid theory for systems of variable range interacting via triangular-well pair potential. **2018**, 265, 337-346 2
- 261 Revisiting electrolyte thermodynamic models: Insights from molecular simulations. **2018**, 64, 3728-3734 13
- 260 Predicting vapor liquid equilibria using density functional theory: A case study of argon. *Journal of Chemical Physics*, **2018**, 148, 224501 3.9 8
- 259 Investigating adsorption- and diffusion selectivity of CO₂ and CH₄ from air on zeolitic imidazolate Framework-78 using molecular simulations. **2019**, 274, 266-276 15
- 258 United atom forcefield for vapor-liquid equilibrium (VLE) properties of cyclic and polycyclic compounds from Monte Carlo simulations. *Fluid Phase Equilibria*, **2019**, 481, 28-43 2.5 8
- 257 The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation. **2019**, 45, 48
- 256 Phase Behavior and Capillary Condensation Hysteresis of Carbon Dioxide in Mesopores. **2019**, 35, 11291-11298 21
- 255 Equation of state and force fields for Feynman-Hibbs-corrected Mie fluids. I. Application to pure helium, neon, hydrogen, and deuterium. *Journal of Chemical Physics*, **2019**, 151, 064508 3.9 12
- 254 Obtaining Soft Matter Models of Proteins and their Phase Behavior. **2019**, 2039, 209-228 2
- 253 From a Liquid to a Crystal without Going through a First-Order Phase Transition: Determining the Free Energy of Melting with Glassy Intermediates. *Journal of Physical Chemistry B*, **2019**, 123, 7740-7747 3.4 0
- 252 CO₂ sorption in triethyl(butyl)phosphonium 2-cyanopyrrolide ionic liquid via first principles simulations. **2019**, 292, 111323 3
- 251 Thermodynamic properties and anomalous behavior of double-Gaussian core model potential fluids. **2019**, 100, 012112 3

250	Fully a priori prediction of the vapor-liquid equilibria of Ar, Kr, and Xe from ab initio two-body plus three-body interatomic potentials. <i>Journal of Chemical Physics</i> , 2019 , 151, 034509	3.9	7
249	Molecular simulation data for the vapor-liquid phase equilibria of binary mixtures of HFO-1123 with R-32, R-1234yf, R-1234ze(E), R-134a and CO and their modelling by the PCP-SAFT equation of state. 2019 , 25, 104014		1
248	On the liquid–vapour coexistence curve in a Lennard–Jones fluid. <i>Molecular Physics</i> , 2019 , 117, 3550-3555	1.7	2
247	Phase Behavior of Grafted Polymer Nanocomposites from Field-Based Simulations. 2019 , 52, 5110-5121		16
246	Coexistence calculation using the isothermal-isochoric integration method. <i>Fluid Phase Equilibria</i> , 2019 , 501, 112236	2.5	2
245	Calculation of phase diagrams in the multithermal-multibaric ensemble. <i>Journal of Chemical Physics</i> , 2019 , 150, 244119	3.9	16
244	Improving the efficiency of Monte Carlo simulations of ions using expanded grand canonical ensembles. <i>Journal of Chemical Physics</i> , 2019 , 151, 144109	3.9	1
243	Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. 2019 , 59, 4248-4265		40
242	Effect of Pulverization on the Microporous and Ultramicroporous Structures of Coal Using Low-Pressure CO ₂ Adsorption. 2019 , 33, 10611-10621		10
241	Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers. 2019 , 9,		24
240	Solubility of Water in Hydrogen at High Pressures: A Molecular Simulation Study. 2019 , 64, 4103-4115		16
239	Molecular Simulation Studies on Vapor-Liquid Equilibria and Thermal Decomposition of Working Fluids [A Review]. 2019 , 158, 5263-5268		1
238	Thermodynamic properties of the 3D Lennard-Jones/spline model. <i>Molecular Physics</i> , 2019 , 117, 3754-3769	1.7	9
237	Three archetypical classes of macromolecular regulators of protein liquid-liquid phase separation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019 , 116, 19474-19483	11.5	47
236	Prediction of phase equilibria and Gibbs free energies of transfer using molecular exchange Monte Carlo in the Gibbs ensemble. <i>Fluid Phase Equilibria</i> , 2019 , 486, 106-118	2.5	4
235	Vapor–Liquid Equilibrium Simulations of Hydrocarbons Using Molecular Dynamics with Long-Range Lennard-Jones Interactions. 2019 , 33, 848-858		15
234	Modeling and Simulations of Polymers: A Roadmap. 2019 , 52, 755-786		161
233	Gas-liquid phase equilibrium of a model Langmuir monolayer captured by a multiscale approach. 2019 , 21, 2295-2306		9

232	Improving the accuracy of computing chemical potentials in CFMCM simulations. <i>Molecular Physics</i> , 2019 , 117, 3493-3508	1.7	10
231	Phase behavior of hydrocarbons in nano-pores. <i>Fluid Phase Equilibria</i> , 2019 , 497, 104-121	2.5	17
230	Trace benzene removal from vinyl acetate with ZIFs: A computational study. 2019 , 1158, 41-46		3
229	Elemental and isotopic fractionation of noble gases in gas and oil under reservoir conditions: Impact of thermodiffusion. 2019 , 42, 61		6
228	Molecular Simulations Probing the Thermophysical Properties of Homogeneously Stretched and Bubbly Water Systems. 2019 , 64, 3755-3771		3
227	Phase Equilibria of Solid and Fluid Phases from Molecular Dynamics Simulations with Equilibrium and Nonequilibrium Free Energy Methods. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3778-3792	6.4	1
226	Dispersion truncation affects the phase behavior of bulk and confined fluids: Coexistence, adsorption, and criticality. <i>Journal of Chemical Physics</i> , 2019 , 150, 154104	3.9	5
225	Open-source molecular modeling software in chemical engineering. 2019 , 23, 99-105		4
224	Compositional Modeling of Crude Oils Using C ₁₀ -C ₃₆ Properties Generated by Molecular Simulation. 2019 , 33, 2967-2980		6
223	Pressure and Temperature Tuning of Gas-Expanded Liquid Structure and Dynamics. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 2915-2924	3.4	2
222	The Influence of Bond Angle on Thermophysical Properties of Three-Center Lennard-Jones Fluids: Computer Simulation and Theory. 2019 , 233, 551-576		2
221	Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. 2019 , 9, e1414		2
220	Pore-Scale Modeling and Simulation in Shale Gas Formations. 2019 , 217-246		1
219	The inhibitory mechanism of aurintricarboxylic acid targeting serine/threonine phosphatase Stp1 in <i>Staphylococcus aureus</i> : insights from molecular dynamics simulations. 2019 , 40, 850-858		5
218	Two-body intermolecular potentials from second virial coefficient properties. <i>Journal of Chemical Physics</i> , 2019 , 150, 024503	3.9	7
217	Phase Separation Dynamics of a Binary Fluid with a Closed-Loop Phase Diagram. 2019 , 88, 024007		
216	Direct visualization and molecular simulation of dewpoint pressure of a confined fluid in sub-10 nm slit pores. 2019 , 235, 1216-1223		29
215	GOMC: GPU Optimized Monte Carlo for the simulation of phase equilibria and physical properties of complex fluids. 2019 , 9, 20-27		20

214	Solubility prediction in mixed solvents: A combined molecular simulation and experimental approach. <i>Fluid Phase Equilibria</i> , 2019 , 484, 26-37	2.5	3
213	Vapor-Liquid equilibrium and molecular simulation data for carbon dioxide (CO ₂) + trans-1,3,3,3-tetrafluoroprop-1-ene (R-1234ze(E)) mixture at temperatures from 283.32 to 353.02 K and pressures up to 7.6 MPa. 2019 , 98, 362-371		11
212	Calculation of cross second virial coefficients using ab initio intermolecular potential energy surfaces for dimer H ₂ -N ₂ . 2019 , 517, 208-221		3
211	Thermodynamic Properties of Vapor-Liquid Equilibria from Monte-Carlo Simulation using ab initio Intermolecular Potentials of Systems H ₂ -H ₂ and F ₂ -F ₂ . 2019 , 233, 493-525		1
210	Langevin dynamics simulation with dipole-dipole interactions: Massive performance improvements and advanced analytical integrator. 2019 , 235, 169-178		1
209	Critical temperature determination on a square-well fluid using an adaptation of the microcanonical-ensemble computer simulation method. <i>Molecular Physics</i> , 2020 , 118, e1593534	1.7	2
208	Assessing the Quality of Molecular Simulations for Vapor-Liquid Equilibria: An Analysis of the TraPPE Database. 2020 , 65, 1330-1344		16
207	Parameterization Approach for a Systematic Extension of the Hydrofluoroolefin Force Field to Fluorinated Butenes and Hydrochlorofluoroolefin Compounds. 2020 , 65, 1234-1242		5
206	Digital Fluid Physics-Prediction of phase equilibria for several mixtures of CO ₂ with petroleum fluid systems. 2020 , 187, 106752		5
205	Thermodynamics of two-dimensional molecular fluids: Discrete perturbation theory and Monte Carlo simulations. 2020 , 300, 112293		0
204	Vapor- and Liquid-Phase Adsorption of Alcohol and Water in Silicalite-1 Synthesized in Fluoride Media. 2019 , 66, e16868		4
203	Monte Carlo simulations and perturbation theory for highly correlated fluids: The Lennard-Jones core softened potential case. 2020 , 299, 112201		4
202	Enhancing Water Sampling in Free Energy Calculations with Grand Canonical Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6061-6076	6.4	16
201	Review of recent advances in petroleum fluid properties and their representation. 2020 , 83, 103541		7
200	EV11 phosphorylation at S436 regulates interactions with CtBP1 and DNMT3A and promotes self-renewal. 2020 , 11, 878		1
199	Phase behavior of gelatin/maltodextrin aqueous mixtures studied from a combined experimental and theoretical approach. <i>Fluid Phase Equilibria</i> , 2020 , 524, 112675	2.5	
198	Designing the Morphology of Separated Phases in Multicomponent Liquid Mixtures. 2020 , 125, 218003		11
197	Sorption-induced polymer rearrangement: approaches from molecular modeling. 2020 , 70, 984		7

196	. 2020 ,			8
195	Review and comparison of equations of state for the Lennard-Jones fluid. <i>Fluid Phase Equilibria</i> , 2020 , 523, 112772	2.5		14
194	Multiple linear regression and thermodynamic fluctuations are equivalent for computing thermodynamic derivatives from molecular simulation. <i>Fluid Phase Equilibria</i> , 2020 , 523, 112785	2.5		10
193	Ab initio structure and thermodynamics of the RPBE-D3 water/vapor interface by neural-network molecular dynamics. <i>Journal of Chemical Physics</i> , 2020 , 153, 144710	3.9		13
192	Liquid-Vapor Coexistence and Critical Point of Mg ₂ SiO ₄ From Ab Initio Simulations. 2020 , 47, e2020GL089599	2		
191	Understanding the properties of liquid-crystalline polymers by computational modeling. 2020 , 3, 032008			10
190	Ab Initio Intermolecular Potential Energy Surfaces and Cross Second Virial Coefficients for the Dimer N-NO. <i>ACS Omega</i> , 2020 , 5, 12539-12549	3.9		
189	A Multi-Scale Modeling of Confined Fluid: from Nanopore to Unconventional Reservoir Simulation. 2020 , 193, 107364			3
188	Confinement-Mediated Phase Behavior of Hydrocarbon Fluids: Insights from Monte Carlo Simulations. 2020 , 36, 7277-7288			8
187	Molecular models for phase equilibria of alkanes with air components and combustion products I. Alkane mixtures with nitrogen, CO ₂ and water. <i>Fluid Phase Equilibria</i> , 2020 , 514, 112553	2.5		4
186	Molecular Mechanism of Gas Solubility in Liquid: Constant Chemical Potential Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 5279-5286	6.4		4
185	References. 2020 , 297-315			
184	Liquid-vapour phase diagram and surface tension of the Lennard-Jones core-softened fluid. 2020 , 314, 113539			1
183	Calculation of thermodynamic properties of vapor-liquid equilibria using ab initio intermolecular potential energy surfaces for dimer O ₂ D ₂ . <i>Molecular Physics</i> , 2020 , 118, e1736673	1.7		1
182	Diagram of vapor-liquid equilibria for n-pentane using hybrid Gibbs ensemble Monte Carlo simulation. 2020 , 58, 101-107			
181	Monte Carlo method in two-dimensional materials. 2020 , 149-163			
180	Purely Predictive Vapor-Liquid Equilibrium Properties of 3,3,4,4,4-Pentafluoro-1-butene (HFO-1345fz), 2,3,3,4,4,4-Hexafluoro-1-butene (HFO-1336yf), and trans-1-Chloro-2,3,3,3-tetrafluoropropene (HCFO-1224yd(E)) from Molecular Simulation. 2020 , 65, 4318-4325			4
179	Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions. <i>Journal of Chemical Physics</i> , 2020 , 153, 010903	3.9		16

178	Molecular models for phase equilibria of alkanes with air components and combustion products II. Alkane/Oxygen mixtures. <i>Fluid Phase Equilibria</i> , 2020 , 520, 112650	2.5	0
177	Excess volume, isothermal compressibility, isentropic compressibility and speed of sound of carbon dioxide+n-heptane binary mixture under pressure up to 70 MPa. II. Molecular simulations. 2020 , 164, 104890		3
176	Gibbs Ensemble Monte Carlo Simulation of Fluids in Confinement: Relation between the Differential and Integral Pressures. 2020 , 10,		5
175	Comparing Alchemical Free Energy Estimates to Experimental Values Based on the Ben-Naim Formula: How Much Agreement Can We Expect?. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 840-847	3-4	1
174	Solubility of Nitrogen in Methane, Ethane, and Mixtures of Methane and Ethane at Titan-Like Conditions: A Molecular Dynamics Study. 2020 , 4, 241-248		2
173	Insights into the Gas Adsorption Mechanisms in Metal-Organic Frameworks from Classical Molecular Simulations. 2020 , 378, 14		7
172	Constant chemical potential, pressure and temperature profiles in liquid-vapour equilibrium obtained by spinodal decomposition. <i>Molecular Physics</i> , 2020 , 118, e1711975	1.7	
171	The effect of surface roughness on the phase behavior of colloidal particles. <i>Journal of Chemical Physics</i> , 2020 , 152, 044902	3-9	3
170	Molecular modeling of vapor-liquid equilibrium properties of HFC-161 and its mixture HFC-161+HFO-1234yf. 2020 , 306, 112896		2
169	Optimising the parameters of the Gibbs Ensemble Monte Carlo simulation of phase separation: the role of multiple relaxation times. 2020 , 46, 616-626		1
168	Brick-CFCMC: Open Source Software for Monte Carlo Simulations of Phase and Reaction Equilibria Using the Continuous Fractional Component Method. 2020 , 60, 2678-2682		14
167	Towards Molecular Simulations that are Transparent, Reproducible, Usable By Others, and Extensible (TRUE). <i>Molecular Physics</i> , 2020 , 118,	1.7	12
166	Temperature effects on the spatial distribution of electrolyte mixtures at the aqueous liquid-vapor interface. 2020 , 22, 10792-10801		
165	A Force Field for Poly(oxymethylene) Dimethyl Ethers (OME). <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2517-2528	6.4	3
164	Molecular Mechanism for Azeotrope Formation in Ethanol/Benzene Binary Mixtures through Gibbs Ensemble Monte Carlo Simulation. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 3371-3386	3-4	4
163	Solid-solid phase equilibria in the NaCl-KCl system. <i>Journal of Chemical Physics</i> , 2020 , 152, 144109	3-9	1
162	DL_MONTE: a multipurpose code for Monte Carlo simulation. 2021 , 47, 131-151		10
161	Coupled confined phase behavior and transport of methane in slit nanopores. 2021 , 404, 126502		12

- 160 Effects of Electrolytes on Thermodynamics and Structure of Oligo(ethylene oxide)/Salt Solutions and Liquid-Liquid Equilibria of a Squalane/Tetraethylene Glycol Dimethyl Ether Blend. **2021**, 54, 1120-1136 1
- 159 Gibbs Ensemble Monte Carlo for Reactive Force Fields to Determine the Vapor-Liquid Equilibrium of CO and HO. *Journal of Chemical Theory and Computation*, **2021**, 17, 322-329 6.4 5
- 158 Gibbs ensemble Monte Carlo simulations of the liquid-vapor equilibrium and the critical point of sodium. **2021**, 23, 311-319
- 157 Recent advances in the continuous fractional component Monte Carlo methodology. **2021**, 47, 804-823 14
- 156 Equilibrium properties of penetrable soft spheres. *Molecular Physics*, **2021**, 119, e1802076 1.7 0
- 155 Effect of hard particles on the ferromagnetic transition in dipolar fluids, a simulation study. *Molecular Physics*, **2021**, 119, e1821920 1.7
- 154 Gibbs-ensemble Monte Carlo simulation of H₂-He mixtures. **2021**, 103, 013307 2
- 153 Thermodynamic insights into Henry's constant in hyperthermal oxidation of silicon for fabricating optical waveguides. **2021**, 23, 17354-17364
- 152 Adsorption of furan, hexanoic acid, and alkanes in a hierarchical zeolite at reaction conditions: Insights from molecular simulations. **2021**, 48, 101267 2
- 151 Gibbs-ensemble Monte Carlo simulation of H-HO mixtures. **2021**, 23, 12637-12643 0
- 150 Particle size and phase equilibria in classical logarithmic fluid. **2021**, 1740, 012042 1
- 149 Open-source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. **2021**, 67, e17206 6
- 148 Generalized equation of state for fluids: From molecular liquids to colloidal dispersions. *Journal of Chemical Physics*, **2021**, 154, 084902 3.9 1
- 147 A Bidimensional Gay-Berne Calamitic Fluid: Structure and Phase Behavior in Bulk and Strongly Confined Systems. **2021**, 8, 2
- 146 On the Gibbs-Thomson equation for the crystallization of confined fluids. *Journal of Chemical Physics*, **2021**, 154, 114711 3.9 4
- 145 First-Principles Grand-Canonical Simulations of Water Adsorption in Proton-Exchanged Zeolites. *Journal of Physical Chemistry C*, **2021**, 125, 6090-6098 3.8 3
- 144 Effects of the repulsive and attractive forces on phase equilibrium and critical properties of two-dimensional non-conformal simple fluids. **2021**, 326, 115234 1
- 143 Effect of Water Content on Thermodynamic Properties of Compressed Hydrogen. **2021**, 66, 2071-2087 4

142	Molecularly Informed Field Theories from Bottom-up Coarse-Graining.. 2021 , 10, 576-583		5
141	First-Principles Simulations of CuCl in High-Temperature Water Vapor. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 4794-4807	3-4	1
140	From predictive modelling to machine learning and reverse engineering of colloidal self-assembly. 2021 , 20, 762-773		20
139	Vapour-Liquid coexistence of carvacrol: a molecular simulation study. <i>Molecular Physics</i> , 2021 , 119,	1-7	0
138	Monte Carlo simulations in the unconstrained ensemble. 2021 , 103, L061303		1
137	Thermodynamic Derivation of Scaling at the Liquid-Vapor Critical Point. 2021 , 23,		
136	Evaluation of Osmotic Virial Coefficients via Restricted Gibbs Ensemble Simulations, with Support from Gas-Phase Mixture Coefficients. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 7262-7272	3-4	0
135	Interatomic Interactions Responsible for the Solid-Liquid and Vapor-Liquid Phase Equilibria of Neon. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 8522-8531	3-4	1
134	The phase diagram of carbon dioxide from correlation functions and a many-body potential. <i>Journal of Chemical Physics</i> , 2021 , 155, 024503	3-9	
133	Database-driven semigrand canonical Monte Carlo method: Application to segregation isotherm on defects in alloys. 2021 , 104, 025310		1
132	Nested sampling for materials. <i>European Physical Journal B</i> , 2021 , 94, 1	1-2	2
131	Adsorption of light gases in covalent organic frameworks: comparison of classical density functional theory and grand canonical Monte Carlo simulations. 2021 , 324, 111263		4
130	LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. 2021 , 271, 108171		315
129	Transferable potential for phase equilibrium of trialkyl borates. 2021 , 339, 116740		0
128	How Molecular Modelling Tools Can Help in Mitigating Climate Change. 2021 , 181-220		0
127	Methods of Computer Simulation. 2021 , 131-193		
126	Monte Carlo Methods for Polymeric Systems. <i>Advances in Chemical Physics</i> , 337-367		5
125	Monte Carlo Methods for Simulating Phase Equilibria of Complex Fluids. <i>Advances in Chemical Physics</i> , 443-460		6

124	Beyond Traditional Effective Intermolecular Potentials and Pairwise Interactions in Molecular Simulation. 2002 , 932-941	3
123	Recent developments in the Monte Carlo simulation of condensed matter. 1992 , 385-410	1
122	Perspective: Free Energies and Phase Equilibria. 2005 , 683-705	4
121	Solvation In Polymers. 2008 , 279-320	6
120	Computer Simulations of Phase Transitions in Liquid Crystals. 1992 , 67-95	5
119	Methods for Examining Phase Equilibria. 2007 , 353-387	3
118	Atomistic Simulation Studies of Polymers and Water. 2006 , 59-65	3
117	Phase Transitions. 2011 , 177-210	1
116	Molecular Simulation: Phase equilibria and confined systems. 1999 , 2-11	1
115	Classical and Quantum Two-Dimensional Fluids in the Gibbs Ensemble. 1994 , 188-192	3
114	Vapor-Liquid Equilibrium. 2010 , 213-240	1
113	Molecular Simulation of Adsorption of Gases on Nanotubes. 2010 , 41-67	7
112	Monte Carlo Simulations. 1990 , 83-123	8
111	Gibbs Ensemble Techniques. 1995 , 463-501	30
110	Numerical Techniques to Study Complex Liquids. 1995 , 357-419	4
109	Modelling Liquid Crystal Structure, Phase Behaviour and Large-Scale Phenomena. 2000 , 73-97	1
108	Phase Transitions without Thermodynamic Limit. 1999 , 31-42	2
107	Computational Studies of Clathrate Hydrates. 1992 , 239-267	3

106	Molecular Simulation of Near-Critical and Supercritical Fluids. 1994 , 387-409		4
105	Molecular Simulation of Phase Equilibria. 1994 , 411-437		3
104	Science: Molecular Simulations and Mesoscale Methods. 2002 , 23-47		1
103	Monte Carlo Simulations. 2017 , 31-82		1
102	Phase transitions in nonadditive hard disc systems: a Gibbs ensemble Monte Carlo Study. 1997 , 104, 166-167		5
101	DIRECT MONTE CARLO SIMULATION OF CHEMICAL EQUILIBRIUM COMPOSITION OF MOLECULAR FLUID MIXTURES UNDER SHOCK CONDITIONS. 1992 , 131-134		1
100	SIMULATION OF MICROPOROUS SYSTEMS: CONFINED FLUIDS IN EQUILIBRIUM AND DIFFUSION IN ZEOLITES. 2001 , 357-443		7
99	Thermodynamic properties and fluid phase equilibrium of natural gas containing CO ₂ and H ₂ O at extreme pressures typically found in pre-salt reservoirs. 2020 , 79, 103337		1
98	Phase Equilibria of Difluoromethane (R32), 1,1,1,2-Tetrafluoroethane (R134a), and trans-1,3,3,3-Tetrafluoro-1-propene (R1234ze(E)) Probed by Experimental Measurements and Monte Carlo Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 739-752	3.9	4
97	Long Range Corrections for Inhomogeneous Simulations of Mie n-m Potential. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4482-4491	6.4	7
96	Effect of the range of particle cohesion on the phase behavior and thermodynamic properties of fluids. <i>Journal of Chemical Physics</i> , 2020 , 153, 244502	3.9	1
95	Combining intermolecular potentials for the prediction of fluid properties: Two-body and three-body interactions. <i>Journal of Chemical Physics</i> , 2020 , 153, 214509	3.9	3
94	On the role of the definition of potential models in Gibbs ensemble phase equilibria simulations of the H ₂ S-pentane mixture. <i>Molecular Physics</i> , 2000 , 98, 1895-1905	1.7	2
93	A transferable potential model for the liquid-vapour equilibria of fluoromethanes. <i>Molecular Physics</i> , 1997 , 92, 825-834	1.7	16
92	Sorption and Diffusion of Small Molecules Using Transition-State Theory. 2004 ,		1
91	Singular value decomposition of the radial distribution function for hard sphere and square well potentials. 2013 , 8, e75792		4
90	Phase equilibria of binary mixtures by molecular simulation and cubic equations of state. 2001 , 18, 149-161		5
89	Molecular Simulations to Research Supercritical Fuel Properties. 2020 , 409-460		2

- 88 Near Critical Coexistence for an AUA Model of Thiophenes. **2008**, 63, 277-282 1
- 87 Approximate equations of the theory of liquids in the statistical thermodynamics of classical liquid systems. **1999**, 169, 625 16
- 86 Molecular distribution functions of stable, metastable and amorphous classical models. **2002**, 172, 647 19
- 85 Monte Carlo Simulation of the Liquid Surface by the Simple Canonical Ensemble, and Estimation of the Heat of Vaporization. **2002**, 3, 73-80
- 84 Phase Behavior in Systems of Large Molecules. **2002**, 247-275
- 83 Some Important Recent Developments of the Monte Carlo Methodology. *Springer Series in Solid-state Sciences*, **2002**, 115-135 0.4
- 82 Monte Carlo Simulations for Complex Fluids.
- 81 Monte Carlo Simulations for Polymers.
- 80 Gibbs Ensemble and Histogram Reweighting Grand Canonical Monte Carlo Methods. **2004**,
- 79 Modelling gas adsorption in slit-pores using Monte Carlo simulation. **2005**,
- 78 References. **2008**, 237-302
- 77 Hierarchical Modeling of Polymeric Systems at Multiple Time and Length Scales. 85-134 1
- 76 Effects of Protein Size on the High-Concentration/Low-Concentration Phase Transition. *Advances in Chemical Physics*, 173-191
- 75 Overview of Computer Simulation Methods. **2013**,
- 74 Molecular Simulation of Vapor-Liquid Equilibrium in Mixed Solvent Electrolyte Solutions. **1993**, 449-460
- 73 Polar / Non-Polar Fluid Mixtures. **1993**, 485-498 1
- 72 On the Non-Solution Region of the Hypernetted Chain and Related Equations for Ionic and Simple Fluids. **1994**, 313-323
- 71 Critical Behavior in Modern Liquid State Theories. **1994**, 325-363

70	Some Important Recent Developments of the Monte Carlo Methodology. <i>Springer Series in Solid-state Sciences</i> , 1997 , 113-132	0.4	
69	Quantum Effects and Phase Transitions in Adsorbed Molecular Layers. 1998 , 325-333		2
68	Theoretical and Simulation Study of Model Protein Solutions. 1999 , 421-436		
67	Field-Based Simulations of Nanostructured Polyelectrolyte Gels. 2016 , 1-9		
66	Vapor-liquid coexisting morphology of all-atom water model through generalized isothermal isobaric ensemble molecular dynamics simulation. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2017 , 66, 136102	0.6	1
65	Nested Sampling for Materials. <i>Springer Theses</i> , 2017 , 61-96	0.1	
64	Liquid-Liquid Phase Separation of Patchy Particles Illuminates Diverse Effects of Regulatory Components on Protein Droplet Formation.		
63	Discotic Dispersions Mediated by Depletion. <i>Springer Theses</i> , 2019 , 85-109	0.1	
62	Absolute chemical potentials for complex molecules in fluid phases: A centroid reference for predicting phase equilibria. <i>Journal of Chemical Physics</i> , 2020 , 153, 214504	3.9	0
61	Methods and Models. <i>Springer Theses</i> , 2020 , 25-33	0.1	
60	Review on metal dissolution characteristics and harmful metals recovery from electronic wastes by supercritical water. <i>Journal of Hazardous Materials</i> , 2021 , 424, 127693	12.8	2
59	Monte Carlo calculations for vapor-liquid phase equilibria in Langmuir monolayers. 1991 , 280-285		1
58	Gaining Insight into the Structure and Dynamics of ClayPolymer Nanocomposite Systems Through Computer Simulation. 2008 , 175-203		
57	Vapor-liquid equilibria and cohesive r interactions. <i>Journal of Chemical Physics</i> , 2020 , 153, 204504	3.9	1
56	Comparison of the GAFF, OPLSAA and CHARMM27 force field for the reproduction of the thermodynamics properties of furfural, 2-methylfuran, 2,5-dimethylfuran and 5-hydroxymethylfurfural. <i>Fluid Phase Equilibria</i> , 2022 , 554, 113331	2.5	0
55	Perspectives for the reconstruction of 3D chromatin conformation using single cell Hi-C data. <i>PLoS Computational Biology</i> , 2021 , 17, e1009546	5	0
54	Computational analysis of homogeneous nucleation and droplet growth applied to natural gas separators. <i>Revista UIS Ingenierías</i> , 2021 , 21,	0.3	0
53	Computational modeling of green hydrogen generation from photocatalytic H ₂ S splitting: Overview and perspectives. <i>Journal of Photochemistry and Photobiology C: Photochemistry Reviews</i> , 2021 , 49, 100456	16.4	1

52 Off-lattice models. **2021**, 243-325

51 Molecular simulations: past, present, and future (a Topical Issue in EPJB). *European Physical Journal B*, **2022**, 95, 1 1.2 2

50 Molecular simulation of methane steam reforming reaction for hydrogen production. *International Journal of Hydrogen Energy*, **2022**, 47, 7569-7585 6.7 1

49 Perspective: Free Energies and Phase Equilibria. **2005**, 683-705 1

48 Vapor-Liquid-Liquid Equilibria of Nitrogen + Ethane by Molecular Simulation. *Industrial & Engineering Chemistry Research*, **2022**, 61, 3104-3112 3.9 0

47 CF Capture and Separation of CF-SF and CF-N Fluid Mixtures Using Selected Carbon Nanoporous Materials and Metal-Organic Frameworks: A Computational Study.. *ACS Omega*, **2022**, 7, 6691-6699 3.9 0

46 Thermoresponsive Ionic Liquid/Water Mixtures: From Nanostructuring to Phase Separation.. *Molecules*, **2022**, 27, 4.8 0

45 1-Bromopropane Capture with Hydrophobic Zeolites: Force Field Development and Molecular Simulations. *Journal of Physical Chemistry C*, **2022**, 126, 5728-5734 3.8 0

44 On the dynamically arrested states of equilibrium and non-equilibrium gels: A comprehensive Brownian Dynamics study.. *Journal of Physics Condensed Matter*, **2022**, 1.8

43 Atomistic simulation framework for molten salt vapor-liquid equilibrium prediction and its application to NaCl.. *Journal of Chemical Physics*, **2022**, 156, 144501 3.9

42 Molecular Simulations for Improved Process Modeling of an Acid Gas Removal Unit. *Fluid Phase Equilibria*, **2022**, 113478 2.5 0

41 Direct free energy evaluation of classical and quantum many-body systems via field-theoretic simulation.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2201804119 11.5 3

40 Vapour-Liquid coexistence of natural phenolic monoterpenoid, thymol: comparison with structural isomer, carvacrol. *Molecular Physics*, 1.7

39 A Simple Model with Wide Applicability for the Determination of Binary Interaction Parameters for Mixtures of n-Alkanes with Carbon Dioxide and Nitrogen. *Industrial & Engineering Chemistry Research*, 3.9 0

38 On the Microscopic Behaviour of the Vapour-Liquid Interface of Methane-Xenon Mixture. *Fluid Phase Equilibria*, **2022**, 113536 2.5

37 Interfacial Properties of Linear Alkane/Nitrogen Binary Mixtures: Molecular Dynamics Vapor-Liquid Equilibrium Simulations. *Journal of Physical Chemistry B*, 3.4

36 SpiDec: Computing Binodals and Interfacial Tension of Biomolecular Condensates From Simulations of Spinodal Decomposition.

35 Drug Discovery by Automated Adaptation of Chemical Structure and Identity. *Journal of Chemical Theory and Computation*, 6.4

34	Calculating adsorption isotherms using the two-phase thermodynamic method and molecular dynamics simulations. <i>Journal of Applied Physics</i> , 2022 , 132, 034701	2.5	0
33	Helium in uranium dioxide: Computer simulation (Review Article). 2022 , 48, 634-644		
32	Computational Modeling of Molecular Mechanics for the Experimentally Inclined.		
31	Modeling the Phase Equilibria of Associating Polymers in Porous Media with Respect to Chromatographic Applications. 2022 , 14, 3182		
30	Extension of the Aggregation-Volume-Bias Monte Carlo Method to the Calculation of Phase Properties of Solid Systems: A Lattice-Based Cluster Approach. 2022 , 126, 5517-5524		
29	Bridging confined phase behavior of CH ₄ -CO ₂ binary systems across scales. 2022 , 105713		1
28	Molecular correlation function integrals for condensed systems with solid-liquid-liquid equilibria. 2022 , 365, 120184		0
27	Modelling Sorption and Transport of Gases in Polymeric Membranes across Different Scales: A Review. 2022 , 12, 857		2
26	Applications of Molecular Dynamics Simulation in Protein Study. 2022 , 12, 844		1
25	Liquid-vapour coexistence line and percolation line of rose water model. 2022 , 120531		0
24	Numerical Techniques for Applications of Analytical Theories to Sequence-Dependent Phase Separations of Intrinsically Disordered Proteins. 2023 , 51-94		1
23	Field-Theoretic Simulation Method to Study the Liquid-Liquid Phase Separation of Polymers. 2023 , 37-49		0
22	Calculating Binodals and Interfacial Tension of Phase-Separated Condensates from Molecular Simulations with Finite-Size Corrections. 2023 , 1-35		0
21	SpiDec: Computing binodals and interfacial tension of biomolecular condensates from simulations of spinodal decomposition. 9,		0
20	Nested Sampling of Materials' Potential Energy Surfaces: Case Study of Zirconium.		0
19	MOLECULAR AND MULTISCALE MODELING: REVIEW ON THE THEORIES AND APPLICATIONS IN CHEMICAL ENGINEERING. 2009 , 3, 205-223		4
18	Accurate determination of solid-liquid equilibria by molecular simulation: behavior of Ne, Ar, Kr, and Xe from low to high pressures.		0
17	Systematic study of vapour-liquid equilibria in binary mixtures of fluids with different polarity from molecular simulations.		0

- 16 Thermodynamics of multipolar Kihara fluids. Results from Monte Carlo simulations and molecular discrete perturbation theory. **2022**, 809, 140171 ○
- 15 Monte Carlo Simulation of NaCl-H₂O Phase Equilibria: Comparison of Classical Force Fields. **2022**, 67, 3661-3671 ○
- 14 Phase Behavior of Methane/n-Butane Binary Mixtures in Organic Nanopores under Bulk Vapor Conditions. **2022**, 36, 14748-14759 ○
- 13 Phase diagrams-why they matter and how to predict them. ○
- 12 Molecular dynamics study of liquid-vapor transition in underwater electrical wire explosion. **2022**, 29, 123503 ○
- 11 Classification methods of pore structures in coal: A review and new insight. **2023**, 204876 ○
- 10 The potential of hydrogen storage in depleted unconventional gas reservoirs: A multiscale modeling study. **2023**, ○
- 9 Molecular Simulation of Hydrogen-Shale Gas System Phase Behavior under Multiscale Conditions: A Molecular-Level Analysis of Hydrogen Storage in Shale Gas Reservoirs. **2023**, 37, 2449-2456 ○
- 8 Continuous fractional component Gibbs ensemble Monte Carlo. **2023**, 91, 235-246 ○
- 7 Equation of state for the Mie ($\bar{\epsilon}_6$) fluid with a repulsive exponent from 11 to 13. **2023**, 158, 084506 ○
- 6 Free energy of critical droplets from the binodal to the spinodal. **2023**, 158, 114108 ○
- 5 Molecular Dynamics Method for Supercritical CO₂ Heat Transfer: A Review. **2023**, 16, 2902 ○
- 4 Monte Carlo Simulations of Water Adsorption in Aluminum Oxide Rod-Based Metal-Organic Frameworks. ○
- 3 A review of GEMC method and its improved algorithms. ○
- 2 Molecular Modeling of Double Retrograde Vaporization Using Monte Carlo Simulations and Equations of State. ○
- 1 Leveraging uncertainty estimates and derivative information in Gaussian process regression for efficient collection and use of molecular simulation data. **2023**, 158, ○