Jayant K Singh

List of Publications by Year
in descending order

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146	4,100	126858	149623
papers	citations	33 h-index	56 g-index

156	156	156	3872
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Integrated docking and enhanced sampling-based selection of repurposing drugs for SARS-CoV-2 by targeting host dependent factors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9897-9908.	2.0	7
2	Tuning the structural properties and chemical activities of graphene and hexagonal boron nitride for efficient adsorption of steroidal pollutants. Applied Surface Science, 2022, 580, 152110.	3.1	6
3	A strategic review of MXenes as emergent building blocks for future two-dimensional materials: recent progress and perspectives. Journal of Materials Chemistry C, 2022, 10, 4096-4123.	2.7	18
4	Mechanistic insights for electrochemical reduction of CO₂ into hydrocarbon fuels over O-terminated MXenes. Catalysis Science and Technology, 2022, 12, 2223-2231.	2.1	22
5	Mechanistic insights of key host proteins and potential repurposed inhibitors regulating SARS<scp>â€CoV</scp>â€2 pathway. Journal of Computational Chemistry, 2022, 43, 1237-1250.	1.5	4
6	Efficient CO₂ Capture and Activation on Novel Two-Dimensional Transition Metal Borides. ACS Applied Materials & Interfaces, 2022, 14, 29703-29710.	4.0	15
7	Insights into the Phase Diagram of Pluronic L64 Using Coarse-Grained Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2022, 126, 4731-4744.	1.2	5
8	Homogeneous nucleation of sheared liquids: advances and insights from simulations and theory. Physical Chemistry Chemical Physics, 2021, 23, 15402-15419.	1.3	9
9	Metadynamics-based enhanced sampling protocol for virtual screening: case study for 3CLpro protein for SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2021, , 1-16.	2.0	7
10	Effects of interfaces on structure and dynamics of water droplets on a graphene surface: A molecular dynamics study. Journal of Chemical Physics, 2021, 154, 164704.	1.2	8
11	A hybrid topological and shape-matching approach for structure analysis. Journal of Chemical Physics, 2021, 154, 154502.	1.2	2
12	Universal Nucleation Behavior of Sheared Systems. Physical Review Letters, 2021, 126, 195702.	2.9	13
13	High-Throughput Screening of Atomic Defects in MXenes for CO₂ Capture, Activation, and Dissociation. ACS Applied Materials & Interfaces, 2021, 13, 35585-35594.	4.0	30
14	Phase Behavior of Pure PSPC and PEGylated Multicomponent Lipid and Their Interaction with Paclitaxel: An All-Atom MD Study. Langmuir, 2021, 37, 10259-10271.	1.6	1
15	Salt-Water System under Diamond Confinement. Journal of Physical Chemistry C, 2021, 125, 22283-22294.	1.5	3
16	Building Unit Extractor for Metalâ€“Organic Frameworks. Journal of Chemical Information and Modeling, 2021, 61, 5827-5840.	2.5	7
17	Molecular Dynamics Study on the Adsorption of UO22+ from an Aqueous Phase: Effect of Grafting Dibenzo Crown Ether and Dicyclohexano Crown Ether on the Polystyrene Surface. Journal of Chemical & Engineering Data, 2020, 65, 1051-1059.	1.0	2
18	Ferrous sulfide and carboxyl-functionalized ferroferric oxide incorporated PVDF-based nanocomposite membranes for simultaneous removal of highly toxic heavy-metal ions from industrial ground water. Journal of Membrane Science, 2020, 593, 117422.	4.1	54

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19	Unraveling the stacking effect and stability in nanocrystalline antimony through DFT. Journal of Physics and Chemistry of Solids, 2020, 136, 109156.	1.9	5
20	A general topological network criterion for exploring the structure of icy nanoribbons and monolayers. Physical Chemistry Chemical Physics, 2020, 22, 3800-3808.	1.3	5
21	Revealing the Limits of Intermolecular Interactions: Molecular Rings of Ferrocene Derivatives on Graphite Surface. Journal of Physical Chemistry Letters, 2020, 11, 297-302.	2.1	3
22	Rationally Designed Semiconducting 2D Surface-Confined Metalâ€“Organic Network. ACS Applied Materials & Interfaces, 2020, 12, 51122-51132.	4.0	3
23	Seeding method for ice nucleation under shear. Journal of Chemical Physics, 2020, 153, 094502.	1.2	11
24	A simple molecular design for tunable two-dimensional imine covalent organic frameworks for optoelectronic applications. Physical Chemistry Chemical Physics, 2020, 22, 21360-21368.	1.3	11
25	High-Throughput Screening of Metalâ€“Organic Frameworks for Ethaneâ€“Ethylene Separation Using the Machine Learning Technique. Energy & Fuels, 2020, 34, 14591-14597.	2.5	26
26	Selective Separation of CO₂ from Flue Gas Using Carbon and Boron Nitride Nanotubes as a Membrane. Energy & Fuels, 2020, 34, 7223-7231.	2.5	7
27	Electronic properties and superior CO2 capture selectivity of metal nitride (XN) and phosphide (XP) (XÂ=ÂAl, Ga and In) sheets. Applied Surface Science, 2020, 527, 146445.	3.1	7
28	Recent Advances in the Carrier Mobility of Two-Dimensional Materials: A Theoretical Perspective. ACS Omega, 2020, 5, 14203-14211.	1.6	130
29	d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations. Journal of Chemical Information and Modeling, 2020, 60, 2169-2177.	2.5	7
30	A review on graphene-based materials for removal of toxic pollutants from wastewater. Soft Materials, 2020, 18, 297-322.	0.8	22
31	Exploring the Anomalous Phase Behavior of High-Pressure Ices in Diamond Confinement. Journal of Physical Chemistry C, 2020, 124, 5460-5468.	1.5	7
32	Validation of Salivary Markers, IL-1Î², IL-8 and Lgals3bp for Detection of Oral Squamous Cell Carcinoma in an Indian Population. Scientific Reports, 2020, 10, 7365.	1.6	20
33	Fe₃O₄-Functionalized Boron Nitride Nanosheets as Novel Adsorbents for Removal of Arsenic(III) from Contaminated Water. ACS Omega, 2020, 5, 10301-10314.	1.6	27
34	A computational study of structural, electronic and carrier mobility of boron and phosphorus/nitrogen co-doped graphene. Physica B: Condensed Matter, 2019, 571, 291-295.	1.3	19
35	Understanding the Adsorption Energetics of Growth Polymorphs of Ferrocene Derivatives: Microscopic Thermal Desorption Analysis. Journal of Physical Chemistry C, 2019, 123, 18488-18494.	1.5	6
36	Electronic Structure of a Semiconducting Imineâ€Covalent Organic Framework. Chemistry - an Asian Journal, 2019, 14, 4645-4650.	1.7	8

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37	Computational Study of the Effect of Functional Groups on Water Adsorption in Mesoporous Carbons: Implications for Gas Adsorption. ACS Applied Nano Materials, 2019, 2, 7103-7113.	2.4	21
38	Study of ice nucleation on silver iodide surface with defects. Molecular Physics, 2019, 117, 3651-3663.	0.8	14
39	Underwater superoleophobic biomaterial based on waste potato peels for simultaneous separation of oil/water mixtures and dye adsorption. Cellulose, 2019, 26, 5497-5511.	2.4	29
40	Adsorption of Gadolinium (Gd³⁺) Ions on the Dibenzo Crown Ether (DBCE) and Dicyclo Hexano Crown Ether (DCHCE) Grafted on the Polystyrene Surface: Insights from All Atom Molecular Dynamics Simulations and Experiments. Journal of Physical Chemistry C, 2019, 123, 12276-12285.	1.5	14
41	Magnetite-Coated Boron Nitride Nanosheets for the Removal of Arsenic(V) from Water. ACS Applied Materials & Interfaces, 2019, 11, 19017-19028.	4.0	50
42	Effect of Ionic Liquid Impregnation in Highly Water-Stable Metalâ€“Organic Frameworks, Covalent Organic Frameworks, and Carbon-Based Adsorbents for Post-combustion Flue Gas Treatment. Energy & Fuels, 2019, 33, 3421-3428.	2.5	27
43	An efficient use of waste PE for hydrophobic surface coating and its application on cotton fibers for oil-water separator. Progress in Organic Coatings, 2019, 131, 301-310.	1.9	30
44	Evaporation induced self-assembly of different shapes and sizes of nanoparticles: A molecular dynamics study. Journal of Chemical Physics, 2019, 150, 044708.	1.2	25
45	Boronâ€“Carbonâ€“Nitride Sheet as a Novel Surface for Biological Applications: Insights from Density Functional Theory. ACS Omega, 2019, 4, 3732-3738.	1.6	29
46	Density Functional Theory Study of Aspirin Adsorption on BCN Sheets and their Hydrogen Evolution Reaction Activity: a Comparative Study with Graphene and Hexagonal Boron Nitride. ChemPhysChem, 2019, 20, 687-694.	1.0	16
47	Ice adhesion mechanism on lubricant-impregnated surfaces using molecular dynamics simulations. Molecular Simulation, 2019, 45, 394-402.	0.9	14
48	Hydrogen adsorption in pyridine bridged porphyrin-covalent organic framework. International Journal of Hydrogen Energy, 2019, 44, 1782-1796.	3.8	38
49	Adsorptive Separation of CO₂ from Multicomponent Mixtures of Flue Gas in Carbon Nanotube Arrays: A Grand Canonical Monte Carlo Study. Energy & Fuels, 2018, 32, 6090-6097.	2.5	17
50	The effect of ionisation of silica nanoparticles on their binding to nonionic surfactants in oilâ€“water system: an atomistic molecular dynamic study. Molecular Physics, 2018, 116, 2022-2031.	0.8	11
51	Extraction of Gd³⁺ and UO₂²⁺ Ions Using Polystyrene Grafted Dibenzo Crown Ether (DB18C6) with Octanol and Nitrobenzene: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2018, 122, 1334-1344.	1.2	12
52	Enhancement of Thermal Energy Transport across the Goldâ€“Graphene Interface Using Nanoscale Defects: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 2113-2121.	1.5	18
53	Nucleation of Aqueous Salt Solutions on Solid Surfaces. Journal of Physical Chemistry C, 2018, 122, 8277-8287.	1.5	14
54	Effect of polystyrene length for the extraction of Gd3+ and UO22+ ions using dicyclohexano crown ether (DCH18C6) with octanol and nitrobenzene: A molecular dynamics study. Journal of Molecular Liquids, 2018, 271, 166-174.	2.3	6

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55	Formation patterns of water clusters in CMK-3 and CMK-5 mesoporous carbons: a computational recognition study. Physical Chemistry Chemical Physics, 2018, 20, 17093-17104.	1.3	8
56	Ice Nucleation on a Graphite Surface in the Presence of Nanoparticles. Journal of Physical Chemistry C, 2018, 122, 19056-19066.	1.5	7
57	Treatment of Flue Gas using Graphene Sponge: A Simulation Study. Journal of Physical Chemistry C, 2018, 122, 14654-14664.	1.5	12
58	A grand canonical Monte Carlo study of SO2 capture using functionalized bilayer graphene nanoribbons. Journal of Chemical Physics, 2017, 146, 044704.	1.2	12
59	Janus Gold Nanoparticles from Nanodroplets of Alkyl Thiols: A Molecular Dynamics Study. Langmuir, 2017, 33, 3056-3067.	1.6	10
60	Fabrication of durable super-repellent surfaces on cotton fabric with liquids of varying surface tension: Low surface energy and high roughness. Applied Surface Science, 2017, 416, 639-648.	3.1	51
61	Fabrication of durable superhydrophobic coatings on cotton fabrics with photocatalytic activity by fluorine-free chemical modification for dual-functional water purification. New Journal of Chemistry, 2017, 41, 4618-4628.	1.4	69
62	Adsorption and Separation of N₂/CH₄/CO₂/SO₂ Gases in Disordered Carbons Obtained Using Hybrid Reverse Monte Carlo Simulations. Journal of Physical Chemistry C, 2017, 121, 13457-13473.	1.5	36
63	Separation of Ethanol and Water Using Graphene and Hexagonal Boron Nitride Slit Pores: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2017, 121, 7867-7880.	1.5	31
64	Simple and green fabrication of recyclable magnetic highly hydrophobic sorbents derived from waste orange peels for removal of oil and organic solvents from water surface. Journal of Environmental Chemical Engineering, 2017, 5, 5250-5259.	3.3	33
65	Thermal conductivity of thermoelectric material Î²-Cu2Se: Implications on phonon thermal transport. Applied Physics Letters, 2017, 111, .	1.5	9
66	An interaction potential to study the thermal structure evolution of a thermoelectric material: Î²â€Cu₂Se. Journal of Computational Chemistry, 2017, 38, 2161-2170.	1.5	20
67	A coarse-grain molecular dynamics study of oilâ€“water interfaces in the presence of silica nanoparticles and nonionic surfactants. Journal of Chemical Physics, 2017, 146, 204702.	1.2	19
68	Removal of Pb(II) Ion Using PAMAM Dendrimer Grafted Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Study. Journal of Physical Chemistry A, 2017, 121, 9320-9329.	1.1	16
69	Striped gold nanoparticles: New insights from molecular dynamics simulations. Journal of Chemical Physics, 2016, 144, 244710.	1.2	12
70	Interfacial behavior of nonionic Tween 20 surfactant at oilâ€“water interfaces in the presence of different types of nanoparticles. RSC Advances, 2016, 6, 113307-113314.	1.7	27
71	Understanding adsorption of CO₂, N₂, CH₄ and their mixtures in functionalized carbon nanopipe arrays. Physical Chemistry Chemical Physics, 2016, 18, 14007-14016.	1.3	23
72	Ice nucleation on nanotextured surfaces: the influence of surface fraction, pillar height and wetting states. Physical Chemistry Chemical Physics, 2016, 18, 26796-26806.	1.3	37

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73	Effect of Different Surfactants on the Interfacial Behavior of the n-Hexaneâ€“Water System in the Presence of Silica Nanoparticles. Journal of Physical Chemistry B, 2016, 120, 7265-7274.	1.2	72
74	Fabrication of zirconia based durable superhydrophobicâ€“superoleophilic fabrics using non fluorinated materials for oilâ€“water separation and water purification. RSC Advances, 2016, 6, 103632-103640.	1.7	60
75	Scaling of granular temperature in vibro-fluidized grains. Physics of Fluids, 2016, 28, .	1.6	14
76	Removal of heavy metal ions using functionalized graphene membranes: a molecular dynamics study. RSC Advances, 2016, 6, 63190-63199.	1.7	45
77	Molecular dynamics study of wetting behavior of grafted thermo-responsive PNIPAAm brushes. Soft Matter, 2016, 12, 3093-3102.	1.2	18
78	Adsorption and Condensation of SO₂ in Double-Walled Carbon Nanotube Arrays Studied by Monte Carlo Simulations and Simple Analytical Models. Journal of Physical Chemistry C, 2016, 120, 7510-7521.	1.5	12
79	Adsorption and separation of binary and ternary mixtures of SO₂, CO₂ and N₂ by ordered carbon nanotube arrays: grand-canonical Monte Carlo simulations. Physical Chemistry Chemical Physics, 2016, 18, 4112-4120.	1.3	30
80	Dewetting dynamics of a gold film on graphene: implications for nanoparticle formation. Faraday Discussions, 2016, 186, 153-170.	1.6	9
81	Double-walled carbon nanotube array for CO2 and SO2 adsorption. Journal of Chemical Physics, 2015, 143, 124701.	1.2	37
82	CO₂ Adsorption on Charged Carbon Nanotube Arrays: A Possible Functional Material for Electric Swing Adsorption. Journal of Physical Chemistry C, 2015, 119, 15232-15239.	1.5	38
83	Molecular simulation of shale gas adsorption and diffusion in inorganic nanopores. Molecular Simulation, 2015, 41, 414-422.	0.9	114
84	Structure of Mixed Self-Assembled Monolayers on Gold Nanoparticles at Three Different Arrangements. Journal of Physical Chemistry C, 2015, 119, 3199-3209.	1.5	28
85	Removal of Heavy Metal Ions Using a Functionalized Single-Walled Carbon Nanotube: A Molecular Dynamics Study. Journal of Physical Chemistry A, 2015, 119, 8349-8358.	1.1	127
86	Ice and water droplets on graphite: A comparison of quantum and classical simulations. Journal of Chemical Physics, 2014, 141, 204701.	1.2	13
87	Localization and stretching of polymer chains at the junction of two surfaces. Journal of Chemical Physics, 2014, 140, 204909.	1.2	3
88	Melting transition of Lennard-Jones fluid in cylindrical pores. Journal of Chemical Physics, 2014, 140, 204703.	1.2	8
89	On the characterization of crystallization and ice adhesion on smooth and rough surfaces using molecular dynamics. Applied Physics Letters, 2014, 104, 021603.	1.5	31
90	Wetting transition of nanodroplets of water on textured surfaces: a molecular dynamics study. Molecular Simulation, 2014, 40, 458-468.	0.9	63

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91	Polymer directed aggregation and dispersion of anisotropic nanoparticles. Soft Matter, 2014, 10, 1823.	1.2	28
92	Wetting Transition of the Ethanolâ€“Water Droplet on Smooth and Textured Surfaces. Journal of Physical Chemistry C, 2014, 118, 4113-4121.	1.5	45
93	Oscillatory Melting Temperature of Stockmayer Fluid in Slit Pores. Journal of Physical Chemistry C, 2014, 118, 20848-20857.	1.5	2
94	Structure and Dynamics of n-Alkanol Monolayers on a Mica Surface. Journal of Physical Chemistry C, 2014, 118, 6809-6819.	1.5	8
95	Structural and dynamical properties of Li+-dibenzo-18-crown-6(DB18C6) complex in pure solvents and at the aqueous-organic interface. Journal of Molecular Modeling, 2014, 20, 2413.	0.8	21
96	Effects of Electric Field on the Vaporâ€“Liquid Equilibria of Nanoconfined Methanol and Ethanol. Journal of Chemical & Engineering Data, 2014, 59, 3090-3097.	1.0	8
97	Adsorption of gas-like molecules to self-aligned square-well fluid channels under confinement of chemically patterned substrates. Applied Nanoscience (Switzerland), 2013, 3, 179-187.	1.6	10
98	Preparation of novel carbon microfiber/carbon nanofiber-dispersed polyvinyl alcohol-based nanocomposite material for lithium-ion electrolyte battery separator. Materials Science and Engineering C, 2013, 33, 1702-1709.	3.8	19
99	Melting transition of confined Lennard-Jones solids in slit pores. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	32
100	Coarse-grain molecular dynamics simulations of nanoparticle-polymer melt: Dispersion vs. agglomeration. Journal of Chemical Physics, 2013, 138, 144901.	1.2	41
101	Effect of confinement on the solid-liquid coexistence of Lennard-Jones Fluid. Journal of Chemical Physics, 2013, 139, 174706.	1.2	11
102	A comparative study of critical temperature estimation of atomic fluid and chain molecules using fourth-order Binder cumulant and simplified scaling laws. Molecular Simulation, 2013, 39, 154-159.	0.9	7
103	Axial segregation of horizontally vibrated binary granular mixtures in an offset-Christmas tree channel. , 2013, , .		0
104	Understanding Carbon Dioxide Adsorption in Carbon Nanotube Arrays: Molecular Simulation and Adsorption Measurements. Journal of Physical Chemistry C, 2013, 117, 13492-13501.	1.5	61
105	Surface phase transitions of multiple-site associating fluids. Molecular Physics, 2012, 110, 1241-1248.	0.8	7
106	From microhydration to bulk hydration of Sr2+ metal ion: DFT, MP2 and molecular dynamics study. Journal of Molecular Liquids, 2012, 172, 110-118.	2.3	20
107	Effect of Electric Field on Water Confined in Graphite and Mica Pores. Journal of Physical Chemistry C, 2012, 116, 17594-17603.	1.5	25
108	Molecular dynamics study of vaporâ€“liquid equilibria and transport properties of sodium and lithium based on EAM potentials. Fluid Phase Equilibria, 2012, 313, 16-24.	1.4	22

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109	Surface Phase Transition of Associating Fluids on Functionalized Surfaces. Journal of Physical Chemistry C, 2011, 115, 17861-17869.	1.5	10
110	Phase Transitions of Water in Graphite and Mica Pores. Journal of Physical Chemistry C, 2011, 115, 12448-12457.	1.5	41
111	Wetting transition of water on graphite and boron-nitride surfaces: A molecular dynamics study. Fluid Phase Equilibria, 2011, 302, 310-315.	1.4	71
112	Effect of pore morphology on vaporâ€“liquid phase transition and crossover behavior of critical properties from 3D to 2D. Fluid Phase Equilibria, 2011, 300, 182-187.	1.4	105
113	Vapourâ€“liquid phase equilibria of simple fluids confined in patterned slit pores. Molecular Simulation, 2011, 37, 350-360.	0.9	8
114	Surface electrophoresis of ds-DNA across orthogonal pair of surfaces. Applied Physics Letters, 2011, 98, 164102.	1.5	13
115	INVESTIGATING BRIDGE-LIKE STRUCTURES IN A SQUARE-WELL BINARY MIXTURE USING NVT MONTE CARLO SIMULATION. International Journal of Nanoscience, 2011, 10, 329-333.	0.4	10
116	Phase transitions in nanoconfined fluids: The evidence from simulation and theory. AICHE Journal, 2010, 56, 842-848.	1.8	39
117	Phase transition and crossover behavior of colloidal fluids under confinement. Chemical Physics Letters, 2010, 494, 182-187.	1.2	8
118	Prewetting transitions of one site associating fluids. Journal of Chemical Physics, 2010, 132, 144501.	1.2	10
119	Direct determination of fluid-solid coexistence of square-well fluids confined in narrow cylindrical hard pores. Journal of Chemical Physics, 2010, 132, 224504.	1.2	14
120	Molecular Simulation Study of Vaporâ^'Liquid Critical Properties of a Simple Fluid in Attractive Slit Pores: Crossover from 3D to 2D. Journal of Physical Chemistry B, 2010, 114, 4283-4292.	1.2	45
121	Molecular Simulation: Can it Help in the Development of Micro and Nano Devices?. , 2010, , 309-331.		1
122	Characterization of fluid-solid phase transition of hard-sphere fluids in cylindrical pore via molecular dynamics simulation. Journal of Chemical Physics, 2009, 130, 164511.	1.2	20
123	Quasi-2D and prewetting transitions of square-well fluids on a square-well substrate. Molecular Physics, 2009, 107, 2189-2200.	0.8	10
124	Vapor-liquid critical and interfacial properties of square-well fluids in slit pores. Journal of Chemical Physics, 2009, 130, 214707.	1.2	42
125	Virial coefficients of hard-core attractive Yukawa fluids. Fluid Phase Equilibria, 2009, 285, 36-43.	1.4	16
126	Axial segregation in horizontally vibrated granular materials: A numerical study. KSCE Journal of Civil Engineering, 2009, 13, 289-296.	0.9	0

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127	Virial coefficients and inversion curve of simple and associating fluids. Fluid Phase Equilibria, 2009, 279, 47-55.	1.4	15
128	Vaporâ˜'Liquid Phase Coexistence, Critical Properties, and Surface Tension of Confined Alkanes. Journal of Physical Chemistry C, 2009, 113, 7170-7180.	1.5	265
129	Surface tension and vapourâ€"liquid phase coexistence of variable-range hard-core attractive Yukawa fluids. Molecular Simulation, 2009, 35, 880-887.	0.9	17
130	Synthesis of anion exchange polystyrene membranes for the electrolysis of sodium chloride. AICHE Journal, 2008, 54, 940-949.	1.8	17
131	The effects of interaction range, porosity and molecular association on the phase equilibrium of a fluid confined in a disordered porous media. Molecular Physics, 2008, 106, 2277-2288.	0.8	7
132	Thin-thick surface phase coexistence and boundary tension of the square-well fluid on a weak attractive surface. Journal of Chemical Physics, 2008, 128, 044708.	1.2	14
133	Characterization of mono- and divacancy in fcc and hcp hard-sphere crystals. Journal of Chemical Physics, 2008, 128, 134514.	1.2	14
134	Interface mixing behaviour of Lennard-Jones FCC (100) thin film. Molecular Physics, 2008, 106, 2417-2423.	0.8	0
135	Molecular Simulation Study of Vapor-Liquid Equilibrium of Morse Fluids. Chemical Product and Process Modeling, 2007, 2, .	0.5	4
136	Surface tension and vapor-liquid phase coexistence of confined square-well fluid. Journal of Chemical Physics, 2007, 126, 024702.	1.2	68
137	Higher-Order Virial Coefficients of Water Models. Journal of Physical Chemistry B, 2007, 111, 11463-11473.	1.2	78
138	Calculation of Phase Coexistence Properties and Surface Tensions of n-Alkanes with Grand-Canonical Transition-Matrix Monte Carlo Simulation and Finite-Size Scaling. Journal of Physical Chemistry B, 2006, 110, 1369-1376.	1.2	91
139	Vaporâ€"liquid phase coexistence curves for Morse fluids. Fluid Phase Equilibria, 2006, 248, 1-6.	1.4	64
140	Molecular Simulation Study of the Effect of Pressure on the Vaporâ˜'Liquid Interface of the Square-Well Fluid. Langmuir, 2005, 21, 4218-4226.	1.6	9
141	Mayer Sampling: Calculation of Cluster Integrals using Free-Energy Perturbation Methods. Physical Review Letters, 2004, 92, 220601.	2.9	156
142	Molecular simulation study of effect of molecular association on vapor-liquid interfacial properties. Journal of Chemical Physics, 2004, 121, 9574-9580.	1.2	30
143	Molecular Simulation Study of the Vaporâ€"Liquid Interfacial Behavior of a Dimer-forming Associating Fluid. Molecular Simulation, 2004, 30, 343-351.	0.9	21
144	Surface tension and vaporâ€"liquid phase coexistence of the square-well fluid. Journal of Chemical Physics, 2003, 119, 3405-3412.	1.2	134

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145	Appropriate methods to combine forward and reverse free-energy perturbation averages. Journal of Chemical Physics, 2003, 118, 2977-2984.	1.2	174
146	Pressure induced phase diagram of double-layer ice under confinement: A first-principles study. Physical Chemistry Chemical Physics, 0, , .	1.3	2