Shiqi Zhou

List of Publications by Year
in descending order

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130 papers	2,039 citations	257357 24 h-index	395590 33 g-index
131 all docs	131 docs citations	131 times ranked	359 citing authors

#	Article	IF	Citations
1	A density functional theory based on the universality of the free energy density functional. Journal of Chemical Physics, 2000, 112, 8079-8082.	1.2	73
2	Thermodynamic perturbation theory in fluid statistical mechanics. Physical Review E, 2006, 74, 031119.	0.8	67
3	Progress in the Perturbation Approach in Fluid and Fluid-Related Theories. Chemical Reviews, 2009, 109, 2829-2858.	23.0	63
4	High-order direct correlation functions of uniform fluids and their application to the high-order perturbative density functional theory. Physical Review E, 2000, 61, 2704-2711.	0.8	54
5	A simple weighted-density-functional method: Test and its application to hard sphere fluid in spherical cavity. Journal of Chemical Physics, 1999, 110, 2140-2144.	1.2	43
6	Fifth-order thermodynamic perturbation theory of uniform and nonuniform fluids. Physical Review E, 2008, 77, 041110.	0.8	43
7	Formally `exact' first-order Taylor series expansion for density functional theory. New Journal of Physics, 2002, 4, 36-36.	1.2	40
8	Partitioned density functional approach for a Lennard-Jones fluid. Physical Review E, 2003, 68, 061201.	0.8	40
9	Improvement on macroscopic compressibility approximation and beyond. Journal of Chemical Physics, 2006, 125, 144518.	1.2	37
10	Inhomogeneous mixture system: A density functional formalism based on the universality of the free energy density functional. Journal of Chemical Physics, 2000, 113, 8719-8723.	1.2	36
11	Reformulation of liquid perturbation theory for low temperatures. Physical Review E, 2009, 79, 011126.	0.8	32
12	How to make thermodynamic perturbation theory to be suitable for low temperature?. Journal of Chemical Physics, 2009, 130, 054103.	1.2	32
13	Lagrangian theorem-based density functional approach free of adjustable parameter. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 319, 279-284.	0.9	30
14	Classical density functional theory and Monte Carlo simulation study of electric double layer in the vicinity of a cylindrical electrode. Journal of Statistical Mechanics: Theory and Experiment, 2017, 2017, 073207.	0.9	30
15	Effective Electrostatic Interactions Between Two Overall Neutral Surfaces with Quenched Charge Heterogeneity Over Atomic Length Scale. Journal of Statistical Physics, 2017, 169, 1019-1037.	0.5	29
16	Monte Carlo and theoretical calculations of the first four perturbation coefficients in the high temperature series expansion of the free energy for discrete and core-softened potential models. Journal of Chemical Physics, 2013, 138, 244115.	1.2	28
17	Microscopic approach for the site distribution and thermodynamic properties of a single-component polymer subjected to an external field. Physical Review E, 2001, 64, 011112.	0.8	27
18	Analysis of the validity of perturbation density functional theory: Based on extensive simulation for simple fluid at supercritical and subcritical temperature under various external potentials. Journal of Chemical Physics, 2005, 122, 064503.	1.2	27

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19	Thermodynamics and phase behavior of a triangle-well model and density-dependent variety. Journal of Chemical Physics, 2009, 130, 014502.	1.2	27
20	Wetting Transition of Nonpolar Neutral Molecule System on a Neutral and Atomic Length Scale Roughness Substrate. Journal of Statistical Physics, 2018, 170, 979-998.	0.5	27
21	Reformulation of density functional theory for generation of the nonuniform density distribution. Physical Review E, 2001, 63, 061206.	0.8	26
22	A method to incorporate the radial distribution function of bulk fluid into the density functional approximation. Journal of Chemical Physics, 2001, 115, 2212-2218.	1.2	24
23	Perturbation Density Functional Theory for Density Profile of A Nonuniform and Uniform Hard Core Attractive Yukawa Model Fluid. Journal of Physical Chemistry B, 2002, 106, 7674-7680.	1.2	24
24	Third-order thermodynamic perturbation theory for effective potentials that model complex fluids. Physical Review E, 2008, 78, 021503.	0.8	24
25	A new method suitable for calculating accurately wetting temperature over a wide range of conditions: Based on the adaptation of continuation algorithm to classical DFT. Journal of Physics and Chemistry of Solids, 2017, 110, 274-283.	1.9	24
26	Structural and electrical properties of an electric double layer formed inside a cylindrical pore investigated by Monte Carlo and classical density functional theory. Microfluidics and Nanofluidics, 2019, 23, 1.	1.0	24
27	Change of electrostatic potential of mean force between two curved surfaces due to different salt composition, ion valence and size under certain ionic strength. Journal of Physics and Chemistry of Solids, 2016, 89, 53-61.	1.9	23
28	Performance Evaluation of Third-Order Thermodynamic Perturbation Theory and Comparison with Existing Liquid State Theories. Journal of Physical Chemistry B, 2007, 111, 10736-10744.	1.2	22
29	Density Functional Analysis of Like-Charged Attraction between Two Similarly Charged Cylinder Polyelectrolytes. Langmuir, 2013, 29, 12490-12501.	1.6	22
30	Properties of a planar electric double layer under extreme conditions investigated by classical density functional theory and Monte Carlo simulations. Journal of Chemical Physics, 2014, 141, 064701.	1.2	21
31	Solvent granularity in the differential electrical capacitance of supercapacitor and mechanism analysis. Physica A: Statistical Mechanics and Its Applications, 2019, 533, 121905.	1.2	21
32	A new density functional approach to nonuniform Lennard-Jones fluids. Journal of Chemical Physics, 2000, 112, 5242-5243.	1.2	20
33	Transformation from Rogers-Young approximation to the density functional approach for nonuniform fluids:â€ƒNumerical recipe. Physical Review E, 2001, 63, 051203.	0.8	20
34	Accurate and local formulation for thermodynamic properties directly from integral equation method. Theoretical Chemistry Accounts, 2007, 117, 555-564.	0.5	20
35	Study of H2 physical adsorption in single-walled carbon nanotube array. AIP Advances, 2013, 3, .	0.6	20
36	Three-body potential amongst similarly or differently charged cylinder colloids immersed in a simple electrolyte solution. Journal of Statistical Mechanics: Theory and Experiment, 2015, 2015, P11030.	0.9	19

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37	Statistical mechanics study on wetting behaviors of Ne on Mg surface. Journal of Physics and Chemistry of Solids, 2017, 103, 123-131.	1.9	19
38	Thermodynamic properties of fluids with Lennardâ€“Jonesâ€“Gauss potential from computer simulation and the coupling parameter series expansion. Molecular Physics, 2018, 116, 491-506.	0.8	19
39	Capacitance of electrical double layer formed inside a single infinitely long cylindrical pore. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 103203.	0.9	19
40	The First Three Coefficients in the High Temperature Series Expansion of Free Energy for Simple Potential Models with Hard-Sphere Cores and Continuous Tails. Journal of Physical Chemistry B, 2013, 117, 9305-9313.	1.2	18
41	Electrostatic potential of mean force between two curved surfaces in the presence of counterion connectivity. Physical Review E, 2015, 92, 052317.	0.8	18
42	An Approximate Analytic Expression for the Surface Charge Density/Surface Potential Relationship for a Spherical Colloidal Particle. Journal of Colloid and Interface Science, 1998, 208, 347-350.	5.0	17
43	Universal calculational recipe for solvent-mediated potential: based on a combination of integral equation theory and density functional theory. Chemical Physics Letters, 2004, 392, 110-115.	1.2	17
44	Theoretical Investigation about the Possible Consequence of Artificial Discontinuity in Pair Potential Function on Overall Phase Behavior. Journal of Physical Chemistry B, 2009, 113, 8635-8645.	1.2	17
45	Novel anomalies for like-charged attraction between curved surfaces and formulation of a hydrogen bonding style mechanism. AIP Advances, 2013, 3, .	0.6	17
46	Semi-analytical hard sphere reference system theory for solvent-mediated potential (III): test and application to system with general interaction potentials. Chemical Physics Letters, 2004, 399, 315-322.	1.2	16
47	Global and critical test of the perturbation density-functional theory based on extensive simulation of Lennard-Jones fluid near an interface and in confined systems. Journal of Chemical Physics, 2005, 123, 124708.	1.2	16
48	Effects of discreteness of surface charges on the effective electrostatic interactions. Journal of Chemical Physics, 2014, 140, 234704.	1.2	16
49	Thermodynamic properties of diamond and wurtzite model fluids from computer simulation and thermodynamic perturbation theory. Physica A: Statistical Mechanics and Its Applications, 2018, 493, 342-358.	1.2	16
50	Inter-surface effective electrostatic interactions in the presence of surface charge discreteness and solvent granularity. Molecular Physics, 2020, 118, e1778807.	0.8	16
51	Density Functional Theory Based on the Universality Principle and Third-Order Expansion Approximation for Adhesive Hard-Sphere Fluid near Surfaces. Journal of Physical Chemistry B, 2001, 105, 10360-10366.	1.2	15
52	Structure of a Confined Square-Well Fluid. Journal of Physical Chemistry B, 2003, 107, 3585-3590.	1.2	15
53	Perturbative density functional approximation in the view of weighted density concept and beyond. Chemical Physics Letters, 2004, 385, 208-213.	1.2	15
54	Universal calculational recipe for the calculation of solvent-mediated potential: (II) based on density functional theory. Chemical Physics Letters, 2004, 399, 323-330.	1.2	15

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55	Solidâ^'Liquid Phase Transition of the Hard-Core Attractive Yukawa System and Its Colloidal Implication. Journal of Physical Chemistry B, 2004, 108, 8447-8451.	1.2	15
56	Comprehensive investigation about the second order term of thermodynamic perturbation expansion. Journal of Chemical Physics, 2009, 131, 134106.	1.2	15
57	A statistical mechanics study on relationship between nanopore size and energy storage in supercapacitors. Journal of Physics and Chemistry of Solids, 2021, 148, 109705.	1.9	15
58	Employing functional counterpart of Lagrangian theorem to improve on density functional theory for density profile of non-uniform fluids. Chemical Physics, 2003, 289, 309-319.	0.9	14
59	Application of Lagrangian theorem-based density-functional approximation free of adjustable parameters to nonhard-sphere fluid. Journal of Chemical Physics, 2004, 121, 895-901.	1.2	14
60	Isostructural solidâ€“solid transitions in binary asymmetrical hard sphere system: Based on solvent-mediated potential. Journal of Colloid and Interface Science, 2005, 288, 308-312.	5.0	14
61	Low temperature behavior of thermodynamic perturbation theory. Physical Chemistry Chemical Physics, 2009, 11, 11528.	1.3	14
62	Inquiry into thermodynamic behavior of hard sphere plus repulsive barrier of finite height. Journal of Chemical Physics, 2009, 131, 204503.	1.2	14
63	New free energy density functional and application to core-softened fluid. Journal of Chemical Physics, 2010, 132, 194112.	1.2	14
64	Solid phase thermodynamic perturbation theory: Test and application to multiple solid phases. Journal of Chemical Physics, 2007, 127, 084512.	1.2	13
65	Can the second virial coefficient be a predictor for the critical temperature?. Molecular Simulation, 2007, 33, 1187-1191.	0.9	13
66	Liquid theory with high accuracy and broad applicability: Coupling parameter series expansion and non hard sphere perturbation strategy. AIP Advances, 2011, 1, .	0.6	13
67	Effective electrostatic potential between two oppositely charged cylinder rods in primitive model and extended primitive model electrolytes. Journal of Statistical Mechanics: Theory and Experiment, 2019, 2019, 033213.	0.9	13
68	How Ion Size influences Energy Storage in Cylindrical Nanoporous Supercapacitors. Journal of Physical Chemistry C, 2019, 123, 29638-29646.	1.5	13
69	On the statistical mechanics investigation of structure and effective electrostatic force between two solid surfaces in electrolyte dissolved in non-polar solvent. Journal of Statistical Mechanics: Theory and Experiment, 2020, 2020, 073210.	0.9	13
70	Formally Exact Truncated Nonuniform Excess Helmholtz Free Energy Density Functional: Test and Application. Journal of Physical Chemistry B, 2004, 108, 3017-3023.	1.2	12
71	Formalism for calculation of polymer-solvent-mediated potential. Physical Review E, 2006, 74, 011402.	0.8	12
72	Ising model study on effects of solvent electric dipole on ultrananoporous supercapacitor. Chinese Journal of Physics, 2021, 73, 391-405.	2.0	12

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73	Structure of inhomogeneous Lennard-Jones fluid near the critical region and close to the vapor-liquid coexistence curve: Monte Carlo and density-functional theory studies. Physical Review E, 2006, 73, 011202.	0.8	11
74	A new scheme for perturbation contribution in density functional theory and application to solvation force and critical fluctuations. Journal of Chemical Physics, 2009, 131, 134702.	1.2	11
75	A theoretical investigation on the honeycomb potential fluid. Journal of Chemical Physics, 2010, 133, 134107.	1.2	11
76	Effects of interionic non-hard sphere neutral interaction and solvent crowding on differential capacitance curve of electrical double layer. Journal of Chemical Physics, 2019, 151, .	1.2	11
77	Influence of solvent granularity on the effective interactions between two overall neutral surfaces with quenched charge heterogeneity. Journal of Molecular Liquids, 2019, 273, 155-163.	2.3	11
78	Impacts of solvent electric dipole and ion valency on energy storage in ultrananoporous supercapacitor: An ising model study. Journal of Physics and Chemistry of Solids, 2021, 157, 110188.	1.9	11
79	Local Structure and Thermodynamics of a Core-Softened Potential Fluid: Theory and Simulation. ChemPhysChem, 2007, 8, 138-147.	1.0	10
80	Phase behavior of density-dependent pair potentials. Journal of Chemical Physics, 2008, 128, 104511.	1.2	10
81	Going beyond the mean field approximation in classical density functional theory and application to one attractive core-softened model fluid. Journal of Statistical Mechanics: Theory and Experiment, 2010, 2010, P11039.	0.9	10
82	PadÃ© approximant for hard sphere ï¼‹ square well and hard sphere ï¼‹ square well ï¼‹ square shoulder model fluids. Physica A: Statistical Mechanics and Its Applications, 2018, 512, 1260-1277.	1.2	10
83	Investigation about validity of the Derjaguin approximation for electrostatic interactions for a sphere-sphere system. Colloid and Polymer Science, 2019, 297, 623-631.	1.0	10
84	A nonperturbative density functional analysis for nonuniform Lennard-Jones fluid. Journal of Chemical Physics, 2000, 113, 8717-8718.	1.2	9
85	Further investigation about Lagrangian theorem-based density functional approximation: test by non-uniform polymer melt. Chemical Physics, 2005, 310, 129-137.	0.9	9
86	Unusual properties of the electric double layer in an extremely narrow nanotube. A grand canonical Monte Carlo and classical DFT study. Journal of Physics and Chemistry of Solids, 2022, 161, 110440.	1.9	9
87	Density functional theory for nonuniform polymer melts: Based on the universality of the free energy density functional. European Physical Journal E, 2000, 3, 343-353.	0.7	8
88	High-Order Perturbative Density Functional Theory for Nonuniform Fluids with an Attractive Tail near Surfaces. Journal of Colloid and Interface Science, 2001, 242, 152-157.	5.0	8
89	Perturbation density functional theory for nonuniform fluid mixture based on Lagrangian theorem. Chemical Physics, 2004, 297, 171-176.	0.9	8
90	Extending the simple weighted density approximation for a hard-sphere fluid to a Lennardâ€“Jones fluid. Journal of Colloid and Interface Science, 2005, 290, 364-372.	5.0	8

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91	Polymer density functional theory approach based on scaling second-order direct correlation function. Journal of Colloid and Interface Science, 2006, 298, 31-38.	5.0	8
92	Convergence and low temperature adaptability analysis of the high temperature series expansion of the free energy. Journal of Chemical Physics, 2013, 139, 124111.	1.2	8
93	Effective electrostatic forces between two neutral surfaces with atomic scale strip shape surface charge separation. Journal of Molecular Liquids, 2020, 312, 113272.	2.3	8
94	Effective electrostatic forces between two neutral surfaces with surface charge separation: valence asymmetry and dielectric constant heterogeneity. Molecular Physics, 2022, 120, .	0.8	8
95	EXTENDING SIMPLE WEIGHTED DENSITY APPROXIMATION FOR HARD SPHERE FLUID TO LENNARDâ€"JONES FLUID (I): TEST. International Journal of Modern Physics B, 2005, 19, 4701-4721.	1.0	7
96	Sedimentation Equilibrium of Colloidal Suspensions in a Planar Pore Based on Density Functional Theory and the Hard-Core Attractive Yukawa Model. Journal of Physical Chemistry B, 2005, 109, 6397-6404.	1.2	7
97	Further Test of Third Order + Second-Order Perturbation DFT Approach:Â Hard Core Repulsive Yukawa Fluid Subjected to Diverse External Fields. Journal of Physical Chemistry B, 2006, 110, 6924-6932.	1.2	7
98	How to extend hard sphere density functional approximation to nonuniform nonhard sphere fluids: Applicable to both subcritical and supercritical temperature regions. Journal of Chemical Physics, 2006, 124, 144501.	1.2	7
99	Non-hard sphere thermodynamic perturbation theory. Journal of Chemical Physics, 2011, 135, 074103.	1.2	7
100	Excellence of numerical differentiation method in calculating the coefficients of high temperature series expansion of the free energy and convergence problem of the expansion. Journal of Chemical Physics, 2014, 141, 244506.	1.2	7
101	Investigation about suitability of hard core attractive Yukawa potential as a model potential for short-range attractive interactions in colloidal dispersions. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2005, 262, 187-190.	2.3	6
102	DENSITY FUNCTIONAL APPROXIMATION FOR NON-HARD SPHERE FLUIDS SUBJECTED TO EXTERNAL FIELDS. International Journal of Modern Physics B, 2006, 20, 469-493.	1.0	6
103	Surface electrostatic force in presence of dimer counter-ion. Journal of Molecular Liquids, 2021, 328, 115225.	2.3	6
104	Local Solvent Density Augmentation around a Solute in Supercritical Solvent Bath:Â 1. A Mechanism Explanation and a New Phenomenon. Journal of Physical Chemistry B, 2005, 109, 7522-7528.	1.2	5
105	â€˜Exactâ€™ integral equation theory and local formulation for excess thermodynamic properties of hard spheres. Chemical Physics, 2006, 330, 478-485.	0.9	5
106	How critical fluctuations influence adsorption properties of a van der Waals fluid onto a spherical colloidal particle. Theoretical Chemistry Accounts, 2009, 124, 279-294.	0.5	5
107	Non hard sphere thermodynamic perturbation theory over a wide range of temperatures. Journal of Statistical Mechanics: Theory and Experiment, 2011, 2011, P09001.	0.9	5
108	Analytical solutions of nonlinear Poissonâ€"Boltzmann equation for colloidal particles immersed in a general electrolyte solution by homotopy perturbation technique. Colloid and Polymer Science, 2012, 290, 1165-1180.	1.0	5

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109	A comprehensive comparison between thermodynamic perturbation theory and first-order mean spherical approximation: Based on discrete potentials with hard core. Chemical Physics, 2017, 493, 1-11.	0.9	5
110	Statistical mechanics approach to inhomogeneous van der Waals fluids. Molecular Simulation, 2006, 32, 1165-1177.	0.9	4
111	Structural Properties of a Model System with Effective Interparticle Interaction Potential Applicable in Modeling of Complex Fluids. Journal of Physical Chemistry B, 2008, 112, 13862-13872.	1.2	4
112	Local structures of fluid with discrete spherical potential: Theory and grand canonical ensemble Monte Carlo simulation. Journal of Chemical Physics, 2008, 129, 124503.	1.2	4
113	Free Energy Density Functional for Adsorption of Fluids in Nanopores. Langmuir, 2010, 26, 17037-17047.	1.6	4
114	Approximate analytical expressions for electrical potential distribution and surface charge density/surface potential relationship for planar, cylindrical, and spherical entities immersed in a general electrolyte solution. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2011, 385, 28-39.	2.3	4
115	Coupling parameter series expansion for fluid with square-well plus repulsive-square-barrier potential. AIP Advances, 2013, 3, 102103.	0.6	4
116	Ultrananoporous supercapacitor with ionic liquid comprised of two-site cation: an Ising model study (II). Journal Physics D: Applied Physics, 2022, 55, 304005.	1.3	4
117	Influence of ion structure and solvent electric dipole on ultrananoporous supercapacitor: a lattice model study. Physica Scripta, 2022, 97, 085402.	1.2	4
118	SolidÂ–liquid transition of charge-stabilized colloidal dispersions: a single-component structure-function approach. Canadian Journal of Physics, 2004, 82, 357-366.	0.4	3
119	Is perturbation DFT approach applicable to purely repulsive fluids?. Physical Chemistry Chemical Physics, 2006, 8, 4009.	1.3	3
120	Acute effect of trace component on capillary phase transition of n-alkanes. Journal of Statistical Mechanics: Theory and Experiment, 2011, 2011, P05023.	0.9	3
121	Effects of nanoscale surface corrugation on surface-to-surface effective potential. Microfluidics and Nanofluidics, 2013, 14, 859-871.	1.0	3
122	Influences of depletion potential on vapor-liquid critical point metastability. AIP Advances, 2016, 6, 045307.	0.6	3
123	Role of neutral and non-hard sphere interaction in differential capacitance of electrical double-layer. Journal of Molecular Liquids, 2019, 295, 111620.	2.3	3
124	Rapidly convergent procedure to solve the density profile equation in the classical density functional theory. Journal of Computational Chemistry, 2006, 27, 941-947.	1.5	2
125	Local Self-Consistent Ornsteinâ^'Zernike Integral Equation Theory and Application to a Generalized Lennard-Jones Potential. Journal of Physical Chemistry B, 2010, 114, 11525-11534.	1.2	2
126	Approximate analytic solution of the nonlinear Poissonâ€“Boltzmann equation for spherical colloidal particles immersed in a general electrolyte solution. Colloid and Polymer Science, 2012, 290, 1511-1526.	1.0	2

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127	A statistical mechanics investigation about general aspects of wetting transition occurring in nonpolar neutral molecule system with a smooth solid wall. Chemical Physics, 2017, 494, 31-46.	0.9	2
128	Highly accurate and simple analytical approach to nonlinear Poissonâ€“Boltzmann equation. Colloid and Polymer Science, 2013, 291, 879-891.	1.0	1
129	Approximate Analytic Expression of Surface Charge Density/Surface Potential Relationship for a Spherical Colloidal Particle Immersed in a General Electrolyte Solution. Journal of Dispersion Science and Technology, 2015, 36, 1742-1747.	1.3	0
130	Analytical Solution of Modified Poissonâ€“Boltzmann Equation and Application to Cylindrical Nanopore Supercapacitor Energy Storage. Colloid Journal, 2022, 84, 222-242.	0.5	0