List of Publications by Year in descending order

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83 papers	5,395 citations	81839 39 h-index	82499 72 g-index
83 all docs	83 docs citations	83 times ranked	2972 citing authors

#	Article	IF	Citations
1	Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. Journal of Computer-Aided Molecular Design, 2021, 35, 261-269.	1.3	6
2	Predicting 1,9-Decadieneâ^'Water Partition Coefficients Using the 3D-RISM-KH Molecular Solvation Theory. Physchem, 2021, 1, 215-224.	0.5	0
3	Benchmarking Free Energy Calculations in Liquid Aliphatic Ketone Solvents Using the 3D-RISM-KH Molecular Solvation Theory. J, 2021, 4, 604-613.	0.6	1
4	To Pass or Not To Pass: Predicting the Bloodâ€"Brain Barrier Permeability with the 3D-RISM-KH Molecular Solvation Theory. ACS Omega, 2019, 4, 16774-16780.	1.6	28
5	Application of the 3D-RISM-KH molecular solvation theory for DMSO as solvent. Journal of Computer-Aided Molecular Design, 2019, 33, 905-912.	1.3	5
6	Predicting skin permeability using the 3D-RISM-KH theory based solvation energy descriptors for a diverse class of compounds. Journal of Computer-Aided Molecular Design, 2019, 33, 605-611.	1.3	4
7	Performance of 3D-RISM-KH in Predicting Hydration Free Energy: Effect of Solute Parameters. Journal of Physical Chemistry A, 2019, 123, 4087-4093.	1.1	26
8	Enhanced solvation force extrapolation for speeding up molecular dynamics simulations of complex biochemical liquids. Journal of Chemical Physics, 2019, 151, 214102.	1.2	5
9	Computational and Experimental Investigations of the Role of Water and Alcohols in the Desorption of Heterocyclic Aromatic Compounds from Kaolinite in Toluene. Journal of Physical Chemistry C, 2018, 122, 10377-10391.	1.5	4
10	Multiscale methods framework: self-consistent coupling of molecular theory of solvation with quantum chemistry, molecular simulations, and dissipative particle dynamics. Physical Chemistry Chemical Physics, 2018, 20, 2947-2969.	1.3	24
11	Multiscale Modeling of Solvation. , 2017, , 95-139.		17
12	Effective Interactions and Adsorption of Heterocyclic Aromatic Hydrocarbons in Kaolinite Organic Solutions Studied by 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry C, 2017, 121, 22092-22104.	1.5	6
13	A closure relation to molecular theory of solvation for macromolecules. Journal of Physics Condensed Matter, 2016, 28, 404003.	0.7	20
14	Calculation of binding free energy of short double stranded oligonucleotides using MM/3D-RISM-KH approach. Journal of Molecular Liquids, 2015, 201, 68-76.	2.3	14
15	Adsorption of Bitumen Model Compounds on Kaolinite in Liquid and Supercritical Carbon Dioxide Solvents: A Study by Periodic Density Functional Theory and Molecular Theory of Solvation. Energy & Fuels, 2015, 29, 2853-2863.	2.5	12
16	Role of Water in Ligand Binding to Maltose-Binding Protein: Insight from a New Docking Protocol Based on the 3D-RISM-KH Molecular Theory of Solvation. Journal of Chemical Information and Modeling, 2015, 55, 317-328.	2.5	20
17	Electric Interfacial Layer of Modified Cellulose Nanocrystals in Aqueous Electrolyte Solution: Predictions by the Molecular Theory of Solvation. Langmuir, 2015, 31, 7106-7116.	1.6	15
18	Octanolâ€"Water Partition Coefficient from 3D-RISM-KH Molecular Theory of Solvation with Partial Molar Volume Correction. Journal of Physical Chemistry B, 2015, 119, 5588-5597.	1.2	39

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19	MTS-MD of Biomolecules Steered with 3D-RISM-KH Mean Solvation Forces Accelerated with Generalized Solvation Force Extrapolation. Journal of Chemical Theory and Computation, 2015, 11, 1875-1895.	2.3	36
20	Predictive Multiscale Modeling of Nanocellulose Based Materials and Systems. IOP Conference Series: Materials Science and Engineering, 2014, 64, 012040.	0.3	9
21	Computational Study of the Effect of Dispersion Interactions on the Thermochemistry of Aggregation of Fused Polycyclic Aromatic Hydrocarbons as Model Asphaltene Compounds in Solution. Journal of Physical Chemistry A, 2014, 118, 896-908.	1.1	47
22	Dissipative Particle Dynamics with an Effective Pair Potential from Integral Equation Theory of Molecular Liquids. Journal of Physical Chemistry B, 2014, 118, 12034-12049.	1.2	9
23	Moleculeâ€“Surface Recognition between Heterocyclic Aromatic Compounds and Kaolinite in Toluene Investigated by Molecular Theory of Solvation and Thermodynamic and Kinetic Experiments. Journal of Physical Chemistry C, 2014, 118, 23821-23834.	1.5	23
24	Adsorption of Indole on Kaolinite in Nonaqueous Media: Organoclay Preparation and Characterization, and 3D-RISM-KH Molecular Theory of Solvation Investigation. Journal of Physical Chemistry C, 2013, 117, 18556-18566.	1.5	34
25	Multiscale modeling of solvation in chemical and biological nanosystems and in nanoporous materials. Pure and Applied Chemistry, 2013, 85, 159-199.	0.9	58
26	Generalised canonicalâ€“isokinetic ensemble: speeding up multiscale molecular dynamics and coupling with 3D molecular theory of solvation. Molecular Simulation, 2013, 39, 25-48.	0.9	17
27	Plant Biomass Recalcitrance: Effect of Hemicellulose Composition on Nanoscale Forces that Control Cell Wall Strength. Journal of the American Chemical Society, 2013, 135, 19048-19051.	6.6	108
28	Multiple time step molecular dynamics in the optimized isokinetic ensemble steered with the molecular theory of solvation: Accelerating with advanced extrapolation of effective solvation forces. Journal of Chemical Physics, 2013, 139, 244106.	1.2	20
29	Molecular theory of solvation for supramolecules and soft matter structures: application to ligand binding, ion channels, and oligomeric polyelectrolyte gelators. Soft Matter, 2012, 8, 1508-1520.	1.2	44
30	Overcoming the Barrier on Time Step Size in Multiscale Molecular Dynamics Simulation of Molecular Liquids. Journal of Chemical Theory and Computation, 2012, 8, 6-16.	2.3	12
31	Interpretation of atomic motion in flexible molecules: Accelerating molecular dynamics simulations. Physical Review E, 2012, 85, 026706.	0.8	7
32	Efficient treatment of solvation shells in 3D molecular theory of solvation. Journal of Computational Chemistry, 2012, 33, 1478-1494.	1.5	49
33	3D-RISM-KH approach for biomolecular modelling at nanoscale: thermodynamics of fibril formation and beyond. Molecular Simulation, 2011, 37, 718-728.	0.9	16
34	Calculation of Local Water Densities in Biological Systems: A Comparison of Molecular Dynamics Simulations and the 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry B, 2011, 115, 319-328.	1.2	80
35	Multiscale methods for nanochemistry and biophysics in solution. Journal of Molecular Liquids, 2011, 164, 101-112.	2.3	18
36	Spatial Decomposition of Solvation Free Energy Based on the 3D Integral Equation Theory of Molecular Liquid: Application to Miniproteins. Journal of Physical Chemistry B, 2011, 115, 310-318.	1.2	24

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37	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. II. Canonical and isokinetic ensembles. Journal of Chemical Physics, 2011, 135, 234107.	1.2	12
38	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. I. Microcanonical ensemble. Journal of Chemical Physics, 2011, 135, 114110.	1.2	9
39	Structural Water Drives Selfâ€assembly of Organic Rosette Nanotubes and Holds Host Atoms in the Channel. ChemPhysChem, 2010, 11, 361-367.	1.0	43
40	Modeling Solvatochromic Shifts Using the Orbital-Free Embedding Potential at Statistically Mechanically Averaged Solvent Density. Journal of Physical Chemistry A, 2010, 114, 6082-6096.	1.1	84
41	Association Thermodynamics and Conformational Stability of Î²-Sheet Amyloid Î²(17-42) Oligomers: Effects of E22Q (Dutch) Mutation and Charge Neutralization. Biophysical Journal, 2010, 98, 282-296.	0.2	49
42	Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. Journal of Chemical Theory and Computation, 2010, 6, 607-624.	2.3	232
43	An MM/3D-RISM Approach for Ligand Binding Affinities. Journal of Physical Chemistry B, 2010, 114, 8505-8516.	1.2	129
44	Water-Soluble J-Type Rosette Nanotubes with Giant Molar Ellipticity. Journal of the American Chemical Society, 2010, 132, 15136-15139.	6.6	61
45	Thermodynamic dependences of slip length for nanofluidic flows over crystalline surfaces: Predictions of molecular theory of solvation. International Journal of Quantum Chemistry, 2009, 109, 1666-1671.	1.0	6
46	Ab Initio Study of Ionic Liquids by KS-DFT/3D-RISM-KH Theory. Journal of Physical Chemistry B, 2009, 113, 3536-3542.	1.2	43
47	Spatial Decomposition Analysis of the Thermodynamics of Cyclodextrin Complexation. Journal of Chemical Theory and Computation, 2009, 5, 1723-1730.	2.3	24
48	Essential Role of Hydration in Aggregation of Misfolded Prion Proteins: Quantification by Molecular Theory of Solvation. Journal of Toxicology and Environmental Health - Part A: Current Issues, 2009, 72, 1060-1068.	1.1	0
49	Ligand Mapping on Protein Surfaces by the 3D-RISM Theory: Toward Computational Fragment-Based Drug Design. Journal of the American Chemical Society, 2009, 131, 12430-12440.	6.6	109
50	Molecular Recognition in Biomolecules Studied by Statistical-Mechanical Integral-Equation Theory of Liquids. Journal of Physical Chemistry B, 2009, 113, 873-886.	1.2	114
51	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. Journal of Physical Chemistry C, 2008, 112, 6794-6810.	1.5	55
52	Hydration Effects on the HET-s Prion and Amyloid-Î² Fibrillous Aggregates, Studied with Three-Dimensional Molecular Theory of Solvation. Biophysical Journal, 2008, 95, 4540-4548.	0.2	45
53	Modelling of bitumen fragment adsorption on Cu+ and Ag+ exchanged zeolite nanoparticles. Molecular Simulation, 2008, 34, 943-951.	0.9	15
54	Hierarchical Self-Assembly of Organic Prolate Nanospheroids from Hydrophobic Rosette Nanotubes. Langmuir, 2008, 24, 4447-4450.	1.6	34

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55	Molecular theory of hydrodynamic boundary conditions in nanofluidics. Journal of Chemical Physics, 2008, 129, 134701.	1.2	37
56	Theoretical analysis on changes in thermodynamic quantities upon protein folding: Essential role of hydration. Journal of Chemical Physics, 2007, 126, 225102.	1.2	75
57	Molecular Basis for Water-Promoted Supramolecular Chirality Inversion in Helical Rosette Nanotubes. Journal of the American Chemical Society, 2007, 129, 5735-5743.	6.6	184
58	Three-Dimensional Distribution Function Theory for the Prediction of Proteinâ^'Ligand Binding Sites and Affinities:â€‰ Application to the Binding of Noble Gases to Hen Egg-White Lysozyme in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 11585-11591.	1.2	41
59	Evaluation of the SCF Combination of KS-DFT and 3D-RISM-KH; Solvation Effect on Conformational Equilibria, Tautomerization Energies, and Activation Barriers. Journal of Chemical Theory and Computation, 2007, 3, 458-476.	2.3	57
60	Microtubule Stability Studied by Three-Dimensional Molecular Theory of Solvation. Biophysical Journal, 2007, 92, 394-403.	0.2	57
61	Theoretical study of the partial molar volume change associated with the pressureâ€‰induced structural transition of ubiquitin. Protein Science, 2007, 16, 1927-1933.	3.1	53
62	A theoretical analysis on hydration thermodynamics of proteins. Journal of Chemical Physics, 2006, 125, 024911.	1.2	139
63	Self-Consistent Combination of the Three-Dimensional RISM Theory of Molecular Solvation with Analytical Gradients and the Amsterdam Density Functional Package. Journal of Physical Chemistry A, 2006, 110, 6083-6090.	1.1	92
64	Theoretical Study of Volume Changes Accompanying Xenonâ^'Lysozyme Binding:Â Implications for the Molecular Mechanism of Pressure Reversal of Anesthesia. Journal of Physical Chemistry B, 2006, 110, 12149-12154.	1.2	18
65	Locating missing water molecules in protein cavities by the three-dimensional reference interaction site model theory of molecular solvation. Proteins: Structure, Function and Bioinformatics, 2006, 66, 804-813.	1.5	89
66	A molecular theory of liquid interfaces. Physical Chemistry Chemical Physics, 2005, 7, 1785.	1.3	41
67	Helical Rosette Nanotubes with Tunable Stability and Hierarchy. Journal of the American Chemical Society, 2005, 127, 8307-8309.	6.6	134
68	Water Molecules in a Protein Cavity Detected by a Statisticalâ^'Mechanical Theory. Journal of the American Chemical Society, 2005, 127, 15334-15335.	6.6	147
69	Three-dimensional Rism Theory for Molecular Liquids and Solid-Liquid Interfaces. , 2004, , 169-275.		39
70	Microscopic description of a liquidâ€“vapor interface by an inhomogeneous integral equation theory. Chemical Physics Letters, 2004, 397, 368-373.	1.2	13
71	Compressibility oftert-Butyl Alcohol-Water Mixtures: The Rism Theory. Journal of Theoretical and Computational Chemistry, 2003, 02, 193-203.	1.8	37
72	TOWARDS A MOLECULAR THEORY FOR THE VAN DER WAALSâ€“MAXWELL DESCRIPTION OF FLUID PHASE TRANSITIONS. Journal of Theoretical and Computational Chemistry, 2002, 01, 381-406.	1.8	41

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73	Structure of tert-Butyl Alcoholâ^'Water Mixtures Studied by the RISM Theory. Journal of Physical Chemistry B, 2002, 106, 5042-5049.	1.2	126
74	Theoretical study for volume changes associated with the helix-coil transition of peptides. Biopolymers, 2001, 59, 512-519.	1.2	53
75	First-principles realization of a van der Waalsâ€"Maxwell theory for water. Chemical Physics Letters, 2001, 349, 496-502.	1.2	92
76	Theoretical study for partial molar volume of amino acids and polypeptides by the three-dimensional reference interaction site model. Journal of Chemical Physics, 2001, 114, 9506-9511.	1.2	84
77	Liquid structure at metal oxideâ€"water interface: accuracy of a three-dimensional RISM methodology. Chemical Physics Letters, 2000, 320, 186-193.	1.2	18
78	Potentials of mean force of simple ions in ambient aqueous solution. II. Solvation structure from the three-dimensional reference interaction site model approach, and comparison with simulations. Journal of Chemical Physics, 2000, 112, 10403-10417.	1.2	127
79	Potentials of mean force of simple ions in ambient aqueous solution. I. Three-dimensional reference interaction site model approach. Journal of Chemical Physics, 2000, 112, 10391-10402.	1.2	258
80	Solution of three-dimensional reference interaction site model and hypernetted chain equations for simple point charge water by modified method of direct inversion in iterative subspace. Journal of Computational Chemistry, 1999, 20, 928-936.	1.5	224
81	Self-consistent description of a metalâ€"water interface by the Kohnâ€"Sham density functional theory and the three-dimensional reference interaction site model. Journal of Chemical Physics, 1999, 110, 10095-10112.	1.2	608
82	Potential of Mean Force between Two Molecular Ions in a Polar Molecular Solvent: A Study by the Three-Dimensional Reference Interaction Site Model. Journal of Physical Chemistry B, 1999, 103, 7942-7957.	1.2	181
83	Three-dimensional density profiles of water in contact with a solute of arbitrary shape: a RISM approach. Chemical Physics Letters, 1998, 290, 237-244.	1.2	409