Norio Yoshida

List of Publications by Year
in descending order

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94	1,649	304368	329751
papers	citations	22 h-index	37 g-index

102	102	102	1065
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Implementation of solvent polarization in three-dimensional reference interaction-site model self-consistent field theory. Chemical Physics Letters, 2022, 797, 139579.	1.2	3
2	Computational Analysis of the SARS-CoV-2 RBDâ€“ACE2-Binding Process Based on MD and the 3D-RISM Theory. Journal of Chemical Information and Modeling, 2022, 62, 2889-2898.	2.5	4
3	Molecular Recognition and Self-Organization in Life Phenomena Studied by a Statistical Mechanics of Molecular Liquids, the RISM/3D-RISM Theory. Molecules, 2021, 26, 271.	1.7	10
4	A computational method to simulate global conformational changes of proteins induced by cosolvent. Journal of Computational Chemistry, 2021, 42, 552-563.	1.5	4
5	Temperature-responsive morphology formation of a PS-b-PI copolymer: a dissipative particle dynamics simulation study. Soft Matter, 2021, 17, 6248-6258.	1.2	4
6	Modeling the interaction of SARS-CoV-2 binding to the ACE2 receptor via molecular theory of solvation. New Journal of Chemistry, 2021, 45, 15448-15457.	1.4	4
7	Solvation dynamics in electronically polarizable solvents: Theoretical treatment using solvent-polarizable three-dimensional reference interaction-site model theory combined with time-dependent density functional theory. Journal of Chemical Physics, 2021, 154, 044504.	1.2	4
8	Self-Consistent Treatment of Solvation Structure with Electronic Structure Based on 3D-RISM Theory. , 2021, , 487-508.		0
9	Structure and Properties of Supercritical Water: Experimental and Theoretical Characterizations. J, 2021, 4, 698-726.	0.6	5
10	Recent Developments of Computational Methods for pKa Prediction Based on Electronic Structure Theory with Solvation Models. J, 2021, 4, 849-864.	0.6	7
11	A 3D-RISM study of water and potassium ion adsorption in Montmorillonite nanoclay. IOP Conference Series: Materials Science and Engineering, 2020, 773, 012060.	0.3	2
12	Nonequilibrium free-energy profile of charge-transfer reaction in polarizable solvent studied using solvent-polarizable three-dimensional reference interaction-site model theory. Journal of Chemical Physics, 2020, 153, 034502.	1.2	3
13	Applicability of density functional and wave function theories combined with the three-dimensional reference interaction site model self-consistent field method to the dâ€“d transitions of a transition metal aqua complex. IOP Conference Series: Materials Science and Engineering, 2020, 773, 012061.	0.3	0
14	The Reference Interaction Site Model Integrated Calculator (RISMiCal) program package for nano- and biomaterials design. IOP Conference Series: Materials Science and Engineering, 2020, 773, 012062.	0.3	10
15	Residue-Specific Binding Mechanisms of Thioflavin T to a Surface of Flat Î²-Sheets within a Peptide Self-Assembly Mimic. Biochemistry, 2020, 59, 2782-2787.	1.2	13
16	Development of a solvent-polarizable three-dimensional reference interaction-site model theory. Journal of Chemical Physics, 2020, 152, 114108.	1.2	6
17	Biophysics at Kyushu University. Biophysical Reviews, 2020, 12, 245-247.	1.5	3
18	Effect of Molecular Orientational Correlations on Solvation Free Energy Computed by Reference Interaction Site Model Theory. Journal of Chemical Information and Modeling, 2019, 59, 3770-3781.	2.5	24

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19	Î²-sheet elasticity of peptide self-assembly mimic, PSAM, with a grafted sequence characterized by comprehensive analyses of isomorphous crystals. Journal of Molecular Liquids, 2019, 290, 111161.	2.3	5
20	Relation between Anharmonicity of Free-Energy Profile and Spectroscopy in Solvation Dynamics: Differences in Spectral Broadening and Peak Shift in Transient Hole-Burning Spectroscopy Studied by Equilibrium Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2019, 123, 7036-7042.	1.2	4
21	Effects of Water Addition on a Catalytic Fluorination of Dienamine. Molecules, 2019, 24, 3428.	1.7	6
22	Implementation of state-averaged MCSCF method to RISM- and 3D-RISM-SCF schemes. Chemical Physics Letters, 2019, 730, 179-185.	1.2	5
23	Three-Dimensional Reference Interaction Site Model Self-Consistent Field Study on the Coordination Structure and Excitation Spectra of Cu(II)â€“Water Complexes in Aqueous Solution. Journal of Physical Chemistry A, 2019, 123, 3344-3354.	1.1	6
24	Solvated lithium ions in defective Prussian blue. IOP Conference Series: Materials Science and Engineering, 2019, 526, 012032.	0.3	4
25	Distinct ionic adsorption sites in defective Prussian blue: a 3D-RISM study. Physical Chemistry Chemical Physics, 2019, 21, 22569-22576.	1.3	6
26	Selective ion binding by human lysozyme studied by the statistical mechanical integral equation theory. , 2019, , 799-802.		0
27	A new method for finding the minimum free energy pathway of ions and small molecule transportation through protein based on 3D-RISM theory and the string method. Chemical Physics Letters, 2018, 699, 22-27.	1.2	4
28	Theoretical analysis of the domain-swapped dimerization of cytochrome c: An MD and 3D-RISM approach. Journal of Chemical Physics, 2018, 148, 025102.	1.2	7
29	Molecular Mechanism of Depolarization-Dependent Inactivation in W366F Mutant of Kv1.2. Journal of Physical Chemistry B, 2018, 122, 10825-10833.	1.2	4
30	An Atomistic Model of a Precursor State of Light-Induced Channel Opening of Channelrhodopsin. Biophysical Journal, 2018, 115, 1281-1291.	0.2	15
31	Role of Mg²⁺ Ions in DNA Hydrolysis by EcoRV, Studied by the 3D-Reference Interaction Site Model and Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 9061-9075.	1.2	6
32	A computational scheme of pK_a values based on the three-dimensional reference interaction site model self-consistent field theory coupled with the linear fitting correction scheme. Physical Chemistry Chemical Physics, 2018, 20, 27272-27279.	1.3	11
33	Statistical Mechanical Integral Equation Approach to Reveal the Solvation Effect on Hydrolysis Free Energy of ATP and Its Analogue. , 2018, , 69-85.		0
34	Theoretical Study on Oligomerization of Cytochrome c. Journal of Computer Chemistry Japan, 2018, 17, 8-13.	0.0	0
35	Molecular Aspects of Solvation Investigated Using Statistical Mechanics. , 2017, , 963-979.		0
36	A relationship between the force curve measured by atomic force microscopy in an ionic liquid and its density distribution on a substrate. Physical Chemistry Chemical Physics, 2017, 19, 30504-30512.	1.3	21

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37	Role of Solvation in Drug Design as Revealed by the Statistical Mechanics Integral Equation Theory of Liquids. Journal of Chemical Information and Modeling, 2017, 57, 2646-2656.	2.5	39
38	Solvatochromism and preferential solvation of Brooker's merocyanine in waterâ€“methanol mixtures. Journal of Computational Chemistry, 2017, 38, 2411-2419.	1.5	12
39	Size-dependent adsorption sites in a Prussian blue nanoparticle: A 3D-RISM study. Chemical Physics Letters, 2017, 684, 117-125.	1.2	15
40	The ion dependence of carbohydrate binding of CBM36: an MD and 3D-RISM study. Journal of Physics Condensed Matter, 2016, 28, 344005.	0.7	10
41	Theoretical analysis of complex formation of p-carboxybenzeneboronic acid with a monosaccharide. Journal of Molecular Liquids, 2016, 217, 93-98.	2.3	9
42	A 3Dâ€RISM/RISM study of the oseltamivir binding efficiency with the wildâ€type and resistanceâ€associated mutant forms of the viral influenza B neuraminidase. Protein Science, 2016, 25, 147-158.	3.1	37
43	Molecular Aspects of Solvation Investigated Using Statistical Mechanics. , 2016, , 1-17.		0
44	Theory of Molecular Recognition and Structural Fluctuation of Biomolecules. , 2016, , 163-181.		0
45	Three-dimensional reference interaction site model self-consistent field analysis of solvent and substituent effects on the absorption spectra of Brooker's merocyanine. Journal of Computational Chemistry, 2015, 36, 1655-1663.	1.5	7
46	Theoretical analysis of co-solvent effect on the proton transfer reaction of glycine in a waterâ€“acetonitrile mixture. Journal of Chemical Physics, 2015, 142, 204103.	1.2	7
47	Probing â€œambivalentâ€•snug-fit sites in the KcsA potassium channel using three-dimensional reference interaction site model (3D-RISM) theory. Pure and Applied Chemistry, 2014, 86, 97-104.	0.9	12
48	Efficient implementation of the three-dimensional reference interaction site model method in the fragment molecular orbital method. Journal of Chemical Physics, 2014, 140, 214118.	1.2	27
49	Theoretical characterization of the â€œridgeâ€•in the supercritical region in the fluid phase diagram of water. Journal of Chemical Physics, 2014, 140, 104511.	1.2	19
50	Distinct configurations of cations and water in the selectivity filter of the KcsA potassium channel probed by 3D-RISM theory. Journal of Molecular Liquids, 2014, 200, 52-58.	2.3	16
51	Water-mediated forces between the nucleotide binding domains generate the power stroke in an ABC transporter. Chemical Physics Letters, 2014, 616-617, 165-170.	1.2	6
52	Theoretical analysis of salt effect on intramolecular proton transfer reaction of glycine in aqueous NaCl solution. Journal of Molecular Liquids, 2014, 200, 32-37.	2.3	8
53	Massively parallel implementation of 3Dâ€RISM calculation with volumetric 3Dâ€FFT. Journal of Computational Chemistry, 2014, 35, 1347-1355.	1.5	38
54	Extended molecular Ornstein-Zernike integral equation for fully anisotropic solute molecules: Formulation in a rectangular coordinate system. Journal of Chemical Physics, 2013, 139, 084119.	1.2	24

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55	Theoretical Study of Salt Effects on the Dielsâ€“Alder Reaction of Cyclopentadiene with Methyl Vinyl Ketone Using RISM-SCF Theory. Journal of Physical Chemistry B, 2013, 117, 14115-14121.	1.2	11
56	Solvent effect on excited states of merocyanines: A theoretical study using the RISMâ€“SCF method. Chemical Physics Letters, 2013, 583, 69-73.	1.2	7
57	Three-Dimensional Reference Interaction Site Model Self-Consistent Field Study of the Electronic Structure of [Cr(H₂O)₆]³⁺ in Aqueous Solution. Journal of Physical Chemistry A, 2013, 117, 8314-8322.	1.1	8
58	Solvent dependence of Stokes shift for organic soluteâ€“solvent systems: A comparative study by spectroscopy and reference interaction-site modelâ€“self-consistent-field theory. Journal of Chemical Physics, 2013, 139, 094503.	1.2	9
59	Solvent Effects on Electronic Structures of Coumarin 153: Parallel Studies by Means of Spectroscopy and RISM-SCF Calculations. Journal of the Physical Society of Japan, 2012, 81, SA016.	0.7	6
60	Elucidating the Molecular Origin of Hydrolysis Energy of Pyrophosphate in Water. Journal of Chemical Theory and Computation, 2012, 8, 2239-2246.	2.3	16
61	Application of efficient algorithm for solving six-dimensional molecular Ornstein-Zernike equation. Journal of Chemical Physics, 2012, 136, 114106.	1.2	13
62	Placevent: An algorithm for prediction of explicit solvent atom distributionâ€”Application to HIVâ€1 protease and Fâ€ATP synthase. Journal of Computational Chemistry, 2012, 33, 1536-1543.	1.5	128
63	Reply to â€œComment on 'Molecular Selectivity in Aquaporin Channels Studied by the 3D- RISM Theory'â€. Journal of Physical Chemistry B, 2011, 115, 8367-8369.	1.2	3
64	Solvent penetration in photoactive yellow protein R52Q mutant: A theoretical study. Journal of Molecular Liquids, 2011, 164, 120-122.	2.3	5
65	A New Approach for Investigating the Molecular Recognition of Protein: Toward Structure-Based Drug Design Based on the 3D-RISM Theory. Journal of Chemical Theory and Computation, 2011, 7, 3803-3815.	2.3	41
66	Electrolytes in biomolecular systems studied with the 3D-RISM/RISM theory. Interdisciplinary Sciences, Computational Life Sciences, 2011, 3, 290-307.	2.2	10
67	The electronic-structure theory of a large-molecular system in solution: Application to the intercalation of proflavine with solvated DNA. Journal of Molecular Liquids, 2011, 159, 83-92.	2.3	37
68	Affinity of small ligands to myoglobin studied by the 3D-RISM theory. Journal of Molecular Liquids, 2011, 159, 93-98.	2.3	6
69	Molecular Ornstein-Zernike self-consistent-field approach to hydrated electron. Procedia Computer Science, 2011, 4, 1214-1221.	1.2	3
70	Molecular Recognition Explored by a Statistical-Mechanics Theory of Liquids. Current Pharmaceutical Design, 2011, 17, 1740-1757.	0.9	7
71	Statistical mechanics theory of molecular recognition and pharmaceutical design. International Reviews in Physical Chemistry, 2011, 30, 445-478.	0.9	3
72	Functions of Biomolecule Revealed by Statistical Mechanics of Molecular Recognition. Seibutsu Butsuri, 2011, 51, 222-225.	0.0	1

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73	Revisiting the Salt-Induced Conformational Change of DNA with 3D-RISM Theory. Journal of Physical Chemistry B, 2010, 114, 6464-6471.	1.2	29
74	Proton Transport through the Influenza A M2 Channel: Three-Dimensional Reference Interaction Site Model Study. Journal of the American Chemical Society, 2010, 132, 9782-9788.	6.6	49
75	Molecular Selectivity in Aquaporin Channels Studied by the 3D- RISM Theory. Journal of Physical Chemistry B, 2010, 114, 7967-7973.	1.2	23
76	Statistical-Mechanics Theory of Molecular Recognition. , 2010, , 63-87.		0
77	The potential of mean force of water and ions in aquaporin channels investigated by the 3D-RISM method. Journal of Molecular Liquids, 2009, 147, 107-111.	2.3	18
78	Theoretical Study of CO Escaping Pathway in Myoglobin with the 3D-RISM Theory. Journal of the American Chemical Society, 2009, 131, 3852-3853.	6.6	62
79	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
80	A Statistical Mechanics Theory of Molecular Recognition. Biological and Medical Physics Series, 2009, , 187-210.	0.3	1
81	On the Proton Exclusion of Aquaporins:â€‰ A Statistical Mechanics Study. Journal of the American Chemical Society, 2008, 130, 1540-1541.	6.6	61
82	Theoretical Study of Temperature and Solvent Dependence of the Free-Energy Surface of the Intramolecular Electron-Transfer Based on the RISM-SCF Theory:â€‰ Application to the 1,3-Dinitrobenzene Radical Anion in Acetonitrile and Methanol. Journal of Physical Chemistry B, 2008, 112, 433-440.	1.2	24
83	Selective Ion Binding by Protein Probed with the Statistical Mechanical Integral Equation Theory. Journal of Physical Chemistry B, 2007, 111, 4588-4595.	1.2	58
84	The statistical-mechanics study for the distribution of water molecules in aquaporin. Chemical Physics Letters, 2007, 449, 196-201.	1.2	21
85	Conformational Equilibrium of 1,2-Dichloroethane in Water:Â Comparison of PCM and RISM-SCF Methods. Journal of Physical Chemistry B, 2006, 110, 16018-16025.	1.2	15
86	Selective Ion-Binding by Protein Probed with the 3D-RISM Theory. Journal of the American Chemical Society, 2006, 128, 12042-12043.	6.6	110
87	Ab Initio Theoretical Study of Temperature and Density Dependence of Molecular and Thermodynamic Properties of Water in the Entire Fluid Region:Â Autoionization Processes. Journal of Physical Chemistry B, 2006, 110, 8451-8458.	1.2	22
88	A new method to determine electrostatic potential around a macromolecule in solution from molecular wave functions. Journal of Computational Chemistry, 2006, 27, 453-462.	1.5	72
89	Molecular Ornsteinâ€“Zernike approach to the solvent effects on solute electronic structures in solution. Journal of Chemical Physics, 2000, 113, 4974.	1.2	39
90	Control of Dihedral Angle of Mesoâ^'Meso Linked Diporphyrins by Introducing Dioxymethylene Straps of Various Length. Organic Letters, 2000, 2, 2963-2966.	2.4	24

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91	Effect of ion vibration for protonâ€transfer reaction of ammonia cation. Journal of Chemical Physics, 1991, 95, 4136-4141.	1.2	8
92	A facile method for preparation of tâ€butyloxycarbonylamino acid pâ€nitroanilides. International Journal of Peptide and Protein Research, 1990, 36, 197-200.	0.1	21
93	Purification and Characterization of an Acidic Amino Acid Specific Endopeptidase of Streptomyces griseus Obtained from a Commercial Preparation (Pronase). Journal of Biochemistry, 1988, 104, 451-456.	0.9	65
94	Isolation and Some Properties of the Fourth Protomer Species of Taro Trypsin Inhibitor. Agricultural and Biological Chemistry, 1985, 49, 2497-2499.	0.3	0