Toshiko Ichiye

List of Publications by Year
in descending order

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85 papers	2,658 citations	270111 25 h-index	232693 48 g-index
86 all docs	86 docs citations	86 times ranked	3033 citing authors

#	Article	IF	Citations
1	Concentration Dependence of Dynamics and Hydrogen Bonding in Aqueous Solutions of Urea, Methyl-substituted Ureas, and Trimethylamine N-Oxide. Journal of Molecular Liquids, 2022, , 119120.	2.3	2
2	How adding a single methylene to dihydrofolate reductase can change its conformational dynamics. Journal of Chemical Physics, 2021, 154, 165103.	1.2	2
3	Adaptations for Pressure and Temperature in Dihydrofolate Reductases. Microorganisms, 2021, 9, 1706.	1.6	3
4	Pressure Adaptations in Deep-Sea Moritella Dihydrofolate Reductases: Compressibility versus Stability. Biology, 2021, 10, 1211.	1.3	5
5	Understanding how water models affect the anomalous pressure dependence of their diffusion coefficients. Journal of Chemical Physics, 2020, 153, 104510.	1.2	10
6	Dynamical Model for the Counteracting Effects of TrimethylamineN-Oxide on Urea in Aqueous Solutions under Pressure. Journal of Physical Chemistry B, 2020, 124, 1978-1986.	1.2	11
7	Effects of Pressure and Temperature on the Atomic Fluctuations of Dihydrofolate Reductase from a Psychropiezophile and a Mesophile. International Journal of Molecular Sciences, 2019, 20, 1452.	1.8	9
8	Adaptations for pressure and temperature effects on loop motion in Escherichia coli and Moritella profunda dihydrofolate reductase. High Pressure Research, 2019, 39, 225-237.	0.4	6
9	Reduction potential calculations of the Feâ€“S clusters in Thermus thermophilus respiratory complex I. Journal of Computational Chemistry, 2019, 40, 1248-1256.	1.5	2
10	Molecular Dynamics and Neutron Scattering Studies of Potassium Chloride in Aqueous Solution. Journal of Physical Chemistry B, 2019, 123, 10807-10813.	1.2	7
11	Dynamical Effects of Trimethylamine N-Oxide on Aqueous Solutions of Urea. Journal of Physical Chemistry B, 2019, 123, 1108-1115.	1.2	18
12	Diffusion of aqueous solutions of ionic, zwitterionic, and polar solutes. Journal of Chemical Physics, 2018, 148, 222827.	1.2	17
13	Quasiharmonic Analysis of the Energy Landscapes of Dihydrofolate Reductase from Piezophiles and Mesophiles. Journal of Physical Chemistry B, 2018, 122, 5527-5533.	1.2	6
14	Enzymes from piezophiles. Seminars in Cell and Developmental Biology, 2018, 84, 138-146.	2.3	26
15	Extreme biophysics: Enzymes under pressure. Journal of Computational Chemistry, 2017, 38, 1174-1182.	1.5	23
16	Quasiharmonic analysis of protein energy landscapes from pressure-temperature molecular dynamics simulations. Journal of Chemical Physics, 2017, 147, 125103.	1.2	7
17	Building better water models using the shape of the charge distribution of a water molecule. Journal of Chemical Physics, 2017, 147, 194103.	1.2	3
18	Multipole moments of water molecules and the aqueous solvation of monovalent ions. Journal of Molecular Liquids, 2017, 228, 54-62.	2.3	12

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19	A single-site multipole model for liquid water. Journal of Chemical Physics, 2016, 145, 034501.	1.2	14
20	What makes proteins work: exploring life inPâ€“Tâ€“X. Physical Biology, 2016, 13, 063001.	0.8	6
21	Protein dynamics and the allâ€ferrous [F e 4 S 4] cluster in the nitrogenase iron protein. Protein Science, 2016, 25, 12-18.	3.1	8
22	Molecular Multipole Potential Energy Functions for Water. Journal of Physical Chemistry B, 2016, 120, 1833-1842.	1.2	10
23	The Surface Potential of the Waterâ€“Vapor Interface from Classical Simulations. Journal of Physical Chemistry B, 2015, 119, 9114-9122.	1.2	37
24	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. Journal of Chemical Physics, 2015, 142, 064501.	1.2	29
25	The molecular charge distribution, the hydration shell, and the unique properties of liquid water. Journal of Chemical Physics, 2014, 141, 244504.	1.2	11
26	Web-Based Computational Chemistry Education with CHARMMing I: Lessons and Tutorial. PLoS Computational Biology, 2014, 10, e1003719.	1.5	14
27	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. PLoS Computational Biology, 2014, 10, e1003739.	1.5	10
28	Assessment of Quantum Mechanical Methods for Copper and Iron Complexes by Photoelectron Spectroscopy. Journal of Chemical Theory and Computation, 2014, 10, 1283-1291.	2.3	18
29	Identifying sequence determinants of reduction potentials of metalloproteins. Journal of Biological Inorganic Chemistry, 2013, 18, 599-608.	1.1	4
30	Characterizing the effects of the protein environment on the reduction potentials of metalloproteins. Journal of Biological Inorganic Chemistry, 2013, 18, 103-110.	1.1	8
31	Effects of Microcomplexity on Hydrophobic Hydration in Amphiphiles. Journal of the American Chemical Society, 2013, 135, 4918-4921.	6.6	27
32	Calculating standard reduction potentials of [4Feâ€“4S] proteins. Journal of Computational Chemistry, 2013, 34, 576-582.	1.5	17
33	Identifying Residues That Cause pH-Dependent Reduction Potentials. Biochemistry, 2013, 52, 3022-3024.	1.2	4
34	Understanding Rubredoxin Redox Sites by Density Functional Theory Studies of Analogues. Journal of Physical Chemistry A, 2012, 116, 8918-8924.	1.1	7
35	Density functional theory calculations of redox properties of ironâ€“sulphur protein analogues. Molecular Simulation, 2011, 37, 572-590.	0.9	13
36	The large quadrupole of water molecules. Journal of Chemical Physics, 2011, 134, 134501.	1.2	49

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37	Understanding structural effects of multipole moments on aqueous solvation of ions using the soft-sticky dipoleâ€“quadrupoleâ€“octupole water model. Chemical Physics Letters, 2010, 499, 219-225.	1.2	13
38	Solvation of biomolecules by the soft sticky dipoleâ€“quadrupoleâ€“octupole water model. Chemical Physics Letters, 2010, 486, 70-73.	1.2	8
39	Solvation of glucose, trehalose, and sucrose by the soft-sticky dipoleâ€“quadrupoleâ€“octupole water model. Chemical Physics Letters, 2010, 491, 218-223.	1.2	28
40	Fold versus sequence effects on the driving force for proteinâ€mediated electron transfer. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2798-2808.	1.5	17
41	Temperature and pressure dependence of the optimized soft-sticky dipole-quadrupole-octupole water model. Journal of Chemical Physics, 2010, 132, 114511.	1.2	25
42	The Molecular Determinants of the Increased Reduction Potential of the Rubredoxin Domain of Rubrerythrin Relative to Rubredoxin. Biophysical Journal, 2010, 98, 560-568.	0.2	13
43	Optimization of Spin-Unrestricted Density Functional Theory for Redox Properties of Rubredoxin Redox Site Analogues. Journal of Chemical Theory and Computation, 2009, 5, 1361-1368.	2.3	15
44	Insight into Environmental Effects on Bonding and Redox Properties of [4Fe-4S] Clusters in Proteins. Journal of the American Chemical Society, 2009, 131, 5724-5725.	6.6	34
45	Cleavage of [4Feâ”4S]-Type Clusters: Breaking the Symmetry. Journal of Physical Chemistry A, 2009, 113, 5710-5717.	1.1	12
46	Probing Ligand Effects on the Redox Energies of [4Feâ˜4S] Clusters Using Broken-Symmetry Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 5671-5676.	1.1	11
47	Probing the structural effects on the intrinsic electronic and redox properties of [2Feâ€2S]+ clusters, a broken-symmetry density functional theory study. Theoretical Chemistry Accounts, 2007, 117, 275-281.	0.5	11
48	Soft sticky dipole-quadrupole-octupole potential energy function for liquid water: An approximate moment expansion. Journal of Chemical Physics, 2006, 124, 134504.	1.2	52
49	Temperature dependence of diffusion properties of soft sticky dipole water. Chemical Physics Letters, 2006, 421, 166-170.	1.2	9
50	Dynamical properties of the soft sticky dipole-quadrupole-octupole water model: A molecular dynamics study. Journal of Chemical Physics, 2006, 125, 144513.	1.2	41
51	Study of multipole contributions to the structure of water around ions in solution using the soft sticky dipole-quadrupole-octupole (SSDQO) model of water. Journal of Chemical Physics, 2006, 124, 174505.	1.2	20
52	Effects of environment on the structure of Pyrococcus furiosus rubredoxin: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2005, 61, 823-828.	1.5	1
53	The role of backbone stability near Ala44 in the high reduction potential class of rubredoxins. Proteins: Structure, Function and Bioinformatics, 2005, 62, 708-714.	1.5	4
54	Electronic Structure and Intrinsic Redox Properties of [2Feâ˜2S]+Clusters with Tri- and Tetracoordinate Iron Sites. Inorganic Chemistry, 2005, 44, 1202-1204.	1.9	14

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55	The unique hydrogen bonded water in the reduced form of Clostridium pasteurianum rubredoxin and its possible role in electron transfer. Journal of Biological Inorganic Chemistry, 2004, 9, 423-428.	1.1	16
56	Crystallographic studies of V44 mutants of Clostridium pasteurianum rubredoxin: Effects of side-chain size on reduction potential. Proteins: Structure, Function and Bioinformatics, 2004, 57, 618-625.	1.5	17
57	Mechanistic Insight into the Symmetric Fission of [4Feâ^'4S] Analogue Complexes and Implications for Cluster Conversions in Ironâ^'Sulfur Proteins. Journal of Physical Chemistry A, 2004, 108, 6750-6757.	1.1	24
58	Understanding Intramolecular Electron Transfer in Ferredoxin:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 2004, 108, 20435-20441.	1.2	21
59	Direct Measurement of the Hydrogen-Bonding Effect on the Intrinsic Redox Potentials of [4Feâ^'4S] Cubane Complexes. Journal of the American Chemical Society, 2004, 126, 15790-15794.	6.6	48
60	Protein Control of Electron Transfer Rates via Polarization: Molecular Dynamics Studies of Rubredoxin. Biophysical Journal, 2004, 86, 2030-2036.	0.2	13
61	A temperature of maximum density in soft sticky dipole water. Chemical Physics Letters, 2003, 376, 646-652.	1.2	34
62	Probing the Intrinsic Electronic Structure of the Cubane [4Feâ^'4S] Cluster:Â Nature's Favorite Cluster for Electron Transfer and Storage. Journal of the American Chemical Society, 2003, 125, 14072-14081.	6.6	74
63	Combined Quantum Chemistry and Photoelectron Spectroscopy Study of the Electronic Structure and Reduction Potentials of Rubredoxin Redox Site Analogues. Journal of Physical Chemistry A, 2003, 107, 2898-2907.	1.1	39
64	Prediction of Reduction Potential Changes in Rubredoxin: A Molecular Mechanics Approach. Biophysical Journal, 2003, 85, 2818-2829.	0.2	25
65	On the electronic structures of gaseous transition metal halide complexes, FeX4â^' and MX3â^' (M=Mn,) Tj ETQq1 1 0.784314 rgBT /Ov of Chemical Physics, 2003, 119, 8311-8320.	1.2	48
66	Coulomb- and Antiferromagnetic-Induced Fission in Doubly Charged Cubelike Fe-S Clusters. Physical Review Letters, 2002, 89, 163401.	2.9	21
67	Sequence Determination of Reduction Potentials by Cysteinyl Hydrogen Bonds and Peptide Dipoles in [4Fe-4S] Ferredoxins. Biophysical Journal, 2001, 81, 601-613.	0.2	39
68	Leucine 41 is a gate for water entry in the reduction of Clostridium pasteurianum rubredoxin. Protein Science, 2001, 10, 613-621.	3.1	46
69	Interactions of the Rubredoxin Redox Site Analogue [Fe(SCH3)4]2-with Water:Â An Ab Initio Quantum Chemistry Study. Journal of Physical Chemistry B, 2000, 104, 2424-2431.	1.2	6
70	Dynamical properties of the soft sticky dipole model of water: Molecular dynamics simulations. Journal of Chemical Physics, 1999, 111, 2701-2709.	1.2	47
71	Ab Initio Quantum Mechanical Study of Metal Substitution in Analogues of Rubredoxin:Â Implications for Redox Potential Control. Journal of Physical Chemistry B, 1999, 103, 8006-8015.	1.2	12
72	Modulation of the Redox Potential of the [Fe(SCys)4] Site in Rubredoxin by the Orientation of a Peptide Dipoleâ€. Biochemistry, 1999, 38, 14803-14809.	1.2	91

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73	Computational studies of redox potentials of electron transfer proteins. , 1999, , .		7
74	Nonlinear response in ionic solvation: A theoretical investigation. Journal of Chemical Physics, 1998, 109, 1074-1083.	1.2	32
75	Conformational Dependence of the Electronic Properties of [Fe(SCH3)4]-,2-. Journal of Physical Chemistry B, 1997, 101, 3633-3643.	1.2	19
76	Temperature Dependence of the Redox Potential of Rubredoxin from Pyrococcus furiosus:â€‰ A Molecular Dynamics Study. Biochemistry, 1996, 35, 13772-13779.	1.2	27
77	The static dielectric constant of the soft sticky dipole model of liquid water: Monte Carlo simulation. Chemical Physics Letters, 1996, 256, 334-340.	1.2	26
78	Soft Sticky Dipole Potential for Liquid Water:Â A New Model. The Journal of Physical Chemistry, 1996, 100, 2723-2730.	2.9	80
79	Solvent free energy curves for electron transfer reactions: A nonlinear solvent response model. Journal of Chemical Physics, 1996, 104, 7561-7571.	1.2	35
80	Molecular dynamics simulations of rubredoxin fromClostridium pasteurianum: Changes in structure and electrostatic potential duringredox reactions. Proteins: Structure, Function and Bioinformatics, 1995, 22, 154-167.	1.5	55
81	New integral equation theory for primitive model ionic liquids: From electrolytes to molten salts. Journal of Chemical Physics, 1994, 100, 9147-9155.	1.2	13
82	Influence of protein flexibility on the redox potential of rubredoxin: Energy minimization studies. Proteins: Structure, Function and Bioinformatics, 1993, 17, 152-160.	1.5	22
83	Collective motions in proteins: A covariance analysis of atomic fluctuations in molecular dynamics and normal mode simulations. Proteins: Structure, Function and Bioinformatics, 1991, 11, 205-217.	1.5	821
84	Anisotropy and anharmonicity of atomic fluctuations in proteins: implications for x-ray analysis. Biochemistry, 1988, 27, 3487-3497.	1.2	36
85	Anisotropy and anharmonicity of atomic fluctuations in proteins: Analysis of a molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 1987, 2, 236-259.	1.5	75