Hisashi Okumura

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9054220/publications.pdf

Version: 2024-02-01

113 papers	2,362 citations	159525 30 h-index	243529 44 g-index
117 all docs	117 docs citations	117 times ranked	1439 citing authors

#	Article	IF	Citations
1	Liquidâ€“vapor coexistence curves of several interatomic model potentials. Journal of Chemical Physics, 2000, 113, 9162-9168.	1.2	134
2	Explicit symplectic integrators of molecular dynamics algorithms for rigid-body molecules in the canonical, isobaric-isothermal, and related ensembles. Journal of Chemical Physics, 2007, 126, 084103.	1.2	88
3	Temperature and pressure denaturation of chignolin: Folding and unfolding simulation by multibaricâ€multithermal molecular dynamics method. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2397-2416.	1.5	82
4	Amyloid Fibril Disruption by Ultrasonic Cavitation: Nonequilibrium Molecular Dynamics Simulations. Journal of the American Chemical Society, 2014, 136, 10549-10552.	6.6	80
5	Replica-Permutation Method with the Suwaâ€“Todo Algorithm beyond the Replica-Exchange Method. Journal of Chemical Theory and Computation, 2013, 9, 570-581.	2.3	75
6	Chemotactic Adaptation Is Altered by Changes in the Carboxy-Terminal Sequence Conserved among the Major Methyl-Accepting Chemoreceptors. Journal of Bacteriology, 1998, 180, 1862-1868.	1.0	67
7	Hamiltonian replica-permutation method and its applications to an alanine dipeptide and amyloid-Î²(29-42) peptides. Journal of Computational Chemistry, 2013, 34, 2493-2497.	1.5	58
8	Monte Carlo simulations in multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 383, 391-396.	1.2	57
9	Structural and fluctuational difference between two ends of Aβ2 amyloid fibril: MD simulations predict only one end has open conformations. Scientific Reports, 2016, 6, 38422.	1.6	57
10	Nonequilibrium molecular dynamics simulations of a bubble. Physical Review E, 2003, 67, 045301.	0.8	56
11	Equation of state and structural properties of the Weeks-Chandler-Andersen fluid. Journal of Chemical Physics, 2006, 124, 164507.	1.2	56
12	Temperature and Pressure Dependence of Alanine Dipeptide Studied by Multibaricâ^'Multithermal Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 12038-12049.	1.2	55
13	Monte Carlo simulations in generalized isobaric-isothermal ensembles. Physical Review E, 2004, 70, 026702.	0.8	54
14	Molecular dynamics simulations in the multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 391, 248-253.	1.2	54
15	Multibaric-multithermal ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2006, 27, 379-395.	1.5	53
16	Reliable Determination of the Liquid-Vapor Critical Point by theNVTPlus Test Particle Method. Journal of the Physical Society of Japan, 2001, 70, 1990-1994.	0.7	49
17	Replica-exchange method in van der Waals radius space: Overcoming steric restrictions for biomolecules. Journal of Chemical Physics, 2010, 132, 134105.	1.2	46
18	Structural basis of TRPA1 inhibition by HC-030031 utilizing species-specific differences. Scientific Reports, 2016, 6, 37460.	1.6	45

#	Article	IF	Citations
19	Partial multicanonical algorithm for molecular dynamics and Monte Carlo simulations. Journal of Chemical Physics, 2008, 129, 124116.	1.2	44
20	Dimerization Process of Amyloid-Î²(29â€“42) Studied by the Hamiltonian Replica-Permutation Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2014, 118, 11428-11436.	1.2	44
21	Free-energy calculation via mean-force dynamics using a logarithmic energy landscape. Physical Review E, 2012, 85, 066702.	0.8	41
22	Multibaricâ€“Multithermal Molecular Dynamics Simulation of Alanine Dipeptide in Explicit Water. Bulletin of the Chemical Society of Japan, 2007, 80, 1114-1123.	2.0	37
23	Oligomer Formation of Amyloid-Î²(29â€“42) from Its Monomers Using the Hamiltonian Replica-Permutation Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2016, 120, 6555-6561.	1.2	36
24	Effects of a Hydrophilic/Hydrophobic Interface on Amyloid-Î² Peptides Studied by Molecular Dynamics Simulations and NMR Experiments. Journal of Physical Chemistry B, 2019, 123, 160-169.	1.2	36
25	Replica exchange molecular dynamics simulation of chitosan for drug delivery system based on carbon nanotube. Journal of Molecular Graphics and Modelling, 2013, 39, 183-192.	1.3	34
26	Transformation between Î±â€helix and Î²â€sheet structures of one and two polyglutamine peptides in explicit water molecules by replicaâ€exchange molecular dynamics simulations. Journal of Computational Chemistry, 2014, 35, 1430-1437.	1.5	34
27	Generalized-ensemble algorithms for molecular dynamics simulations. Molecular Simulation, 2007, 33, 47-56.	0.9	33
28	Conformational Change of Amyloid-Î² 40 in Association with Binding to GM1-Glycan Cluster. Scientific Reports, 2019, 9, 6853.	1.6	33
29	New formula for the bulk viscosity constructed from the interatomic potential and the pair distribution function. Journal of Chemical Physics, 2002, 116, 7400-7410.	1.2	32
30	Transformation of a design peptide between the Î±-helix and Î²-hairpin structures using a helix-strand replica-exchange molecular dynamics simulation. Physical Chemistry Chemical Physics, 2013, 15, 13852.	1.3	31
31	New expression of the bulk viscosity. Physica A: Statistical Mechanics and Its Applications, 2003, 321, 207-219.	1.2	29
32	Dynamic Views of the Fc Region of Immunoglobulin G Provided by Experimental and Computational Observations. Antibodies, 2019, 8, 39.	1.2	29
33	Simulational analysis of the local structure in liquid germanium under pressure. Physical Review B, 2002, 66, .	1.1	28
34	Liquidâ€“Gas Phase Transitions Studied by Multibaricâ€“Multithermal Monte Carlo Simulations. Journal of the Physical Society of Japan, 2004, 73, 3304-3311.	0.7	28
35	Coulomb replicaâ€exchange method: Handling electrostatic attractive and repulsive forces for biomolecules. Journal of Computational Chemistry, 2013, 34, 622-639.	1.5	27
36	Optimization of partial multicanonical molecular dynamics simulations applied to an alaninedipeptide in explicit water solvent. Physical Chemistry Chemical Physics, 2011, 13, 114-126.	1.3	26

#	Article	IF	Citations
37	Development of isothermal-isobaric replica-permutation method for molecular dynamics and Monte Carlo simulations and its application to reveal temperature and pressure dependence of folded, misfolded, and unfolded states of chignolin. Journal of Chemical Physics, 2017, 147, 184107.	1.2	25
38	Replica-permutation molecular dynamics simulations of an amyloid-Î²(16â€“22) peptide and polyphenols. Chemical Physics Letters, 2020, 758, 137913.	1.2	25
39	Molecular dynamics simulations of amyloid-Î²(16â€“22) peptide aggregation at airâ€“water interfaces. Journal of Chemical Physics, 2020, 152, 095101.	1.2	25
40	Some physical properties of the Weeksâ€“Chandlerâ€“Andersen fluid. Molecular Simulation, 2006, 32, 45-50.	0.9	24
41	Structural basis for promiscuous action of monoterpenes on TRP channels. Communications Biology, 2021, 4, 293.	2.0	23
42	The aspartate chemoreceptor Tar is effectively methylated by binding to the methyltransferase mainly through hydrophobic interaction. Molecular Microbiology, 2000, 36, 132-140.	1.2	21
43	Pressure-Induced Helical Structure of a Peptide Studied by Simulated Tempering Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2013, 4, 2079-2083.	2.1	20
44	Molecular simulations by generalized-ensemble algorithms in isothermalâ€“isobaric ensemble. Biophysical Reviews, 2019, 11, 457-469.	1.5	20
45	Molecular dynamics study of liquidâ€“vapor coexistence curves and supercritical fluids. Physica B: Condensed Matter, 2001, 296, 180-183.	1.3	17
46	Conformational populations of ligandâ€sized molecules by replica exchange molecular dynamics and temperature reweighting. Journal of Computational Chemistry, 2010, 31, 1357-1367.	1.5	17
47	Dynamic properties of SARS-CoV and SARS-CoV-2 RNA-dependent RNA polymerases studied by molecular dynamics simulations. Chemical Physics Letters, 2021, 778, 138819.	1.2	17
48	Replica subâ€permutation method for molecular dynamics and monte carlo simulations. Journal of Computational Chemistry, 2019, 40, 2694-2711.	1.5	16
49	Conformation study of É›-cyclodextrin: Replica exchange molecular dynamics simulations. Carbohydrate Polymers, 2016, 141, 99-105.	5.1	15
50	Cavity Closure of 2-Hydroxypropyl-Î²-Cyclodextrin: Replica Exchange Molecular Dynamics Simulations. Polymers, 2019, 11, 145.	2.0	15
51	Role of Water Molecules and Helix Structure Stabilization in the Laser-Induced Disruption of Amyloid Fibrils Observed by Nonequilibrium Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 4964-4976.	1.2	15
52	Expansion Type of Model Fluids. Journal of the Physical Society of Japan, 2001, 70, 1006-1009.	0.7	14
53	Molecular dynamics of the structural changes of helical peptides induced by pressure. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2970-2981.	1.5	14
54	Approximate Formula for Bulk Viscosity. Journal of the Physical Society of Japan, 2002, 71, 685-688.	0.7	13

#	Article	IF	Citations
55	Structural characterization of HypX responsible for CO biosynthesis in the maturation of NiFe-hydrogenase. Communications Biology, 2019, 2, 385.	2.0	13
56	Comparisons between molecular dynamics and hydrodynamics treatment of nonstationary thermal processes in a liquid. Physical Review E, 2004, 70, 061206.	0.8	12
57	Simulated tempering based on global balance or detailed balance conditions: <scp>S</scp>uwaâ€“<scp>T</scp>odo, heat bath, and <scp>M</scp>etropolis algorithms. Journal of Computational Chemistry, 2015, 36, 2344-2349.	1.5	12
58	Promotion and Inhibition of Amyloid-Î² Peptide Aggregation: Molecular Dynamics Studies. International Journal of Molecular Sciences, 2021, 22, 1859.	1.8	12
59	Comparison of Replica-Permutation Molecular Dynamics Simulations with and without Detailed Balance Condition. Journal of the Physical Society of Japan, 2015, 84, 074801.	0.7	11
60	Dimerization of Î±-Synuclein Fragments Studied by Isothermalâ€“Isobaric Replica-Permutation Molecular Dynamics Simulation. Journal of Chemical Information and Modeling, 2021, 61, 1307-1321.	2.5	11
61	Redox-dependent conformational transition of catalytic domain of protein disulfide isomerase indicated by crystal structure-based molecular dynamics simulation. Chemical Physics Letters, 2015, 618, 203-207.	1.2	10
62	Tardigrade Secretory-Abundant Heat-Soluble Protein Has a Flexible Î²-Barrel Structure in Solution and Keeps This Structure in Dehydration. Journal of Physical Chemistry B, 2021, 125, 9145-9154.	1.2	10
63	Rapid QM/MM approach for biomolecular systems under periodic boundary conditions: Combination of the density-functional tight-binding theory and particle mesh Ewald method. Journal of Computational Chemistry, 2016, 37, 2701-2711.	1.5	9
64	Replica permutation with solute tempering for molecular dynamics simulation and its application to the dimerization of amyloid-Î² fragments. Journal of Chemical Physics, 2022, 156, 084109.	1.2	9
65	Simulational study of liquid germanium under pressure. Journal of Non-Crystalline Solids, 2002, 312-314, 95-98.	1.5	8
66	First derivative of the hard-sphere radial distribution function at contact. Journal of Physics Condensed Matter, 2006, 18, 7553-7558.	0.7	8
67	Decomposition-order effects of time integrator on ensemble averages for the NosÃ©-Hoover thermostat. Journal of Chemical Physics, 2013, 139, 064103.	1.2	8
68	Onâ€theâ€fly reconstruction of freeâ€energy profiles using logarithmic meanâ€force dynamics. Journal of Computational Chemistry, 2013, 34, 1375-1384.	1.5	8
69	Conformational properties of an artificial GM1 glycan cluster based on a metal-ligand complex. Journal of Chemical Physics, 2018, 149, 135101.	1.2	8
70	Classical Molecular Dynamics Simulation to Understand Role of a Zinc Ion for Aggregation of Amyloid-Î² Peptides. Journal of Computer Chemistry Japan, 2018, 17, 76-79.	0.0	8
71	Molecular Dynamics Simulation Studies on the Aggregation of Amyloid-Î² Peptides and Their Disaggregation by Ultrasonic Wave and Infrared Laser Irradiation. Molecules, 2022, 27, 2483.	1.7	8
72	Bulk viscosity in the case of the interatomic potential depending on density. Physical Review E, 2003, 67, 021205.	0.8	7

#	Article	IF	Citations
73	â€œBucket brigadeâ€•using lysine residues in RNA-dependent RNA polymerase of SARS-CoV-2. Biophysical Journal, 2021, 120, 3615-3627.	0.2	7
74	Energetics and kinetics of substrate analog-coupled staphylococcal nuclease folding revealed by a statistical mechanical approach. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 19953-19962.	3.3	6
75	Generalized-Ensemble Algorithms for Simulations of Complex Molecular Systems. , 2012, , 69-101.		6
76	Length Dependence of Polyglycine Conformations in Vacuum. Journal of the Physical Society of Japan, 2011, 80, 094801.	0.7	5
77	Theoretical approaches for dynamical ordering of biomolecular systems. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 212-228.	1.1	5
78	All-Atom Molecular Dynamics Simulation Methods for the Aggregation of Protein and Peptides: Replica Exchange/Permutation and Nonequilibrium Simulations. Methods in Molecular Biology, 2022, 2340, 197-220.	0.4	5
79	Liquid-Vapor Coexistence Curve and Fluid Structure. Progress of Theoretical Physics Supplement, 2000, 138, 253-254.	0.2	4
80	Precise determination of the liquidâ€“vapor critical point by the NVT plus test particle method. Journal of Non-Crystalline Solids, 2002, 312-314, 256-259.	1.5	4
81	Generalized-ensemble molecular dynamics and Monte Carlo algorithms beyond the limit of the multicanonical algorithm. Advances in Natural Sciences: Nanoscience and Nanotechnology, 2010, 1, 033002.	0.7	4
82	Antigen-dependent fluorescence response of anti-c-Myc Quenchbody studied by molecular dynamics simulations. Chemical Physics Letters, 2018, 698, 223-226.	1.2	4
83	Method for liquidâ€“vapor coexistence curves by test-particle insertions in the canonical ensemble. Journal of Non-Crystalline Solids, 2001, 293-295, 715-718.	1.5	3
84	Protein Simulations by Multibaricâ€“Multithermal Molecular Dynamics Algorithm. Journal of the Physical Society of Japan, 2012, 81, SA001.	0.7	3
85	Manifold Correction Method for the NosÃ©â€“Hoover and NosÃ©â€“PoincarÃ© Molecular Dynamics Simulations. Journal of the Physical Society of Japan, 2014, 83, 024003.	0.7	3
86	Examination of Temperature Dependence of Chemical Sputtering on Graphite by Comparing the Langevin and Berendsen Thermostats. Plasma and Fusion Research, 2010, 5, S2020-S2020.	0.3	3
87	Molecular dynamics simulations of amyloid-Î² peptides in heterogeneous environments. Biophysics and Physicobiology, 2022, 19, n/a.	0.5	3
88	Tardigrade Secretory-Abundant Heat-Soluble Protein Varies Entrance Propensity Depending on the Amino-Acid Sequence. Journal of Physical Chemistry B, 2022, 126, 2361-2368.	1.2	3
89	Bulk viscosity in a density-dependent-potential system. Journal of Non-Crystalline Solids, 2002, 312-314, 260-264.	1.5	2
90	Hydrodynamics in a nanoscale liquid: comparisons with molecular dynamics in non-stationary processes. Molecular Physics, 2006, 104, 3751-3756.	0.8	2

#	Article	IF	Citations
91	Stationary temperature profiles in a liquid nanochannel: Comparisons between molecular-dynamics simulation and classical hydrostatics. Physical Review E, 2006, 74, 061201.	0.8	2
92	Cutoff Effect in the NosÃ©â€“PoincarÃ© and NosÃ©â€“Hoover Thermostats. Journal of the Physical Society of Japan, 2013, 82, 034001.	0.7	2
93	Structural dynamics and susceptibility of anti-HIV drugs against HBV reverse transcriptase. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2502-2511.	2.0	2
94	Implementations of replica-permutation and replica sub-permutation methods into LAMMPS. Computer Physics Communications, 2022, 276, 108362.	3.0	2
95	Molecular simulations in the multibaric-multithermal ensembles. Computer Physics Communications, 2005, 169, 317-321.	3.0	1
96	High Pressure Effect on a Helical Peptide Studied by Simulated Tempering Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 611a.	0.2	1
97	Molecular dynamics simulation study on the high-pressure behaviour of an AK16 peptide. Molecular Simulation, 2015, 41, 1035-1040.	0.9	1
98	Structural Changes in Amyloid-Î² by Binding to Glycan Clusters. Seibutsu Butsuri, 2021, 61, 186-188.	0.0	1
99	The Relationship between the Metal-Nonmetal Transition and the Coordination Number in Divalent Systems. Progress of Theoretical Physics Supplement, 2000, 138, 255-256.	0.2	0
100	Multibaricâ€“Multithermal Ensemble Simulation for Simple Liquids. Molecular Simulation, 2004, 30, 847-852.	0.9	0
101	Multibaricâ€“multithermal ensemble simulations for fluid systems. Physica A: Statistical Mechanics and Its Applications, 2005, 350, 150-158.	1.2	0
102	1P585 Explicit Symplectic Molecular Dynamics Simulation for Rigid-Body Molecules in the Canonical Ensemble(27. Molecular dynamics simulation,Poster Session,Abstract,Meeting Program of EABS &) Tj ETQq0 0 0 rgBT /Overlock 10	0.0	0
103	Multibaricâ€“multithermal molecular dynamics simulation: generalized NosÃ©â€“PoincarÃ©â€“Andersen method. Molecular Simulation, 2007, 33, 91-96.	0.9	0
104	3TA5-02 Conformational changes of a peptide induced by temperature and pressure : multibaric-multithermal molecular dynamics simulations(The 47th Annual Meeting of the Biophysical) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.0	0
105	3P071 multibaric-multithermal molecular dynamics simulations of a polyalanine(Protein: Property,The) Tj ETQq1 1 0.784314 rgBT /Over	0.0	0
106	3E1058 Studies on a AÎ² fragment by the Coulomb replica-exchange method(Proteins:Structure,Oral) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.0	0
107	Probing a Non-biaxial Behavior of Infinitely Thin Hard Platelets. Journal of the Physical Society of Japan, 2012, 81, 114003.	0.7	0
108	Nonequilibrium and generalized-ensemble molecular dynamics simulations for amyloid fibril. AIP Conference Proceedings, 2015, , .	0.3	0

#	Article	IF	Citations
109	Replica-permutation method to enhance sampling efficiency. Molecular Simulation, 2015, 41, 1021-1026.	0.9	0
110	Pressure Denaturation of Proteins and Peptides Studied by Molecular Dynamics Simulations. Seibutsu Butsuri, 2016, 56, 212-216.	0.0	0
111	â€ŸComputer Chemistry in Dynamical Ordering of Biomolecular Systems for Creation of Integrated Functionsâ€• Journal of Computer Chemistry Japan, 2018, 17, A1-A2.	0.0	0
112	Involvement of pore helix in voltage-dependent inactivation of TRPM5 channel. Heliyon, 2021, 7, e06102.	1.4	0
113	10.1063/1.5045310.1. , 2018, , .		0