# Hisashi Okumura

List of Publications by Year
in descending order



| 113 | 2,362 | 159573 | 243610 |
|---|---|---|---|
| papers | citations | 30 h-index | 44 g-index |

| 117 | 117 | 117 | 1439 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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. | 3.0 | 9 |
| 2 | Molecular dynamics simulations of amyloid-Î² peptides in heterogeneous environments. Biophysics and Physicobiology, 2022, 19, n/a. | 1.0 | 3 |
| 3 | 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. | 0.9 | 5 |
| 4 | Tardigrade Secretory-Abundant Heat-Soluble Protein Varies Entrance Propensity Depending on the Amino-Acid Sequence. Journal of Physical Chemistry B, 2022, 126, 2361-2368. | 2.6 | 3 |
| 5 | Implementations of replica-permutation and replica sub-permutation methods into LAMMPS. Computer Physics Communications, 2022, 276, 108362. | 7.5 | 2 |
| 6 | 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. | 3.8 | 8 |
| 7 | Structural dynamics and susceptibility of anti-HIV drugs against HBV reverse transcriptase. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2502-2511. | 3.5 | 2 |
| 8 | Structural Changes in Amyloid-Î² by Binding to Glycan Clusters. Seibutsu Butsuri, 2021, 61, 186-188. | 0.1 | 1 |
| 9 | Dimerization of Î±-Synuclein Fragments Studied by Isothermalâ€“Isobaric Replica-Permutation Molecular Dynamics Simulation. Journal of Chemical Information and Modeling, 2021, 61, 1307-1321. | 5.4 | 11 |
| 10 | Promotion and Inhibition of Amyloid-Î² Peptide Aggregation: Molecular Dynamics Studies. International Journal of Molecular Sciences, 2021, 22, 1859. | 4.1 | 12 |
| 11 | Structural basis for promiscuous action of monoterpenes on TRP channels. Communications Biology, 2021, 4, 293. | 4.4 | 23 |
| 12 | 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. | 2.6 | 15 |
| 13 | 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. | 2.6 | 10 |
| 14 | Dynamic properties of SARS-CoV and SARS-CoV-2 RNA-dependent RNA polymerases studied by molecular dynamics simulations. Chemical Physics Letters, 2021, 778, 138819. | 2.6 | 17 |
| 15 | â€œBucket brigadeâ€•using lysine residues in RNA-dependent RNA polymerase of SARS-CoV-2. Biophysical Journal, 2021, 120, 3615-3627. | 0.5 | 7 |
| 16 | Involvement of pore helix in voltage-dependent inactivation of TRPM5 channel. Heliyon, 2021, 7, e06102. | 3.2 | 0 |
| 17 | Replica-permutation molecular dynamics simulations of an amyloid-Î²(16â€“22) peptide and polyphenols. Chemical Physics Letters, 2020, 758, 137913. | 2.6 | 25 |
| 18 | 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. | 7.1 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Molecular dynamics simulations of amyloid-Î²(16â€“22) peptide aggregation at airâ€“water interfaces. Journal of Chemical Physics, 2020, 152, 095101. | 3.0 | 25 |
| 20 | Dynamic Views of the Fc Region of Immunoglobulin G Provided by Experimental and Computational Observations. Antibodies, 2019, 8, 39. | 2.5 | 29 |
| 21 | Replica subâ€permutation method for molecular dynamics and monte carlo simulations. Journal of Computational Chemistry, 2019, 40, 2694-2711. | 3.3 | 16 |
| 22 | Structural characterization of HypX responsible for CO biosynthesis in the maturation of NiFe-hydrogenase. Communications Biology, 2019, 2, 385. | 4.4 | 13 |
| 23 | Cavity Closure of 2-Hydroxypropyl-Î²-Cyclodextrin: Replica Exchange Molecular Dynamics Simulations. Polymers, 2019, 11, 145. | 4.5 | 15 |
| 24 | Molecular simulations by generalized-ensemble algorithms in isothermalâ€“isobaric ensemble. Biophysical Reviews, 2019, 11, 457-469. | 3.2 | 20 |
| 25 | Conformational Change of Amyloid-Î² 40 in Association with Binding to GM1-Glycan Cluster. Scientific Reports, 2019, 9, 6853. | 3.3 | 33 |
| 26 | 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. | 2.6 | 36 |
| 27 | Antigen-dependent fluorescence response of anti-c-Myc Quenchbody studied by molecular dynamics simulations. Chemical Physics Letters, 2018, 698, 223-226. | 2.6 | 4 |
| 28 | Theoretical approaches for dynamical ordering of biomolecular systems. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 212-228. | 2.4 | 5 |
| 29 | â€ŸComputer Chemistry in Dynamical Ordering of Biomolecular Systems for Creation of Integrated Functionsâ€• Journal of Computer Chemistry Japan, 2018, 17, A1-A2. | 0.1 | 0 |
| 30 | Conformational properties of an artificial GM1 glycan cluster based on a metal-ligand complex. Journal of Chemical Physics, 2018, 149, 135101. | 3.0 | 8 |
| 31 | 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. | 0.1 | 8 |
| 32 | 10.1063/1.5045310.1. , 2018, , . | | 0 |
| 33 | 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. | 3.0 | 25 |
| 34 | Structural and fluctuational difference between two ends of Aî² amyloid fibril: MD simulations predict only one end has open conformations. Scientific Reports, 2016, 6, 38422. | 3.3 | 57 |
| 35 | 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. | 3.3 | 9 |
| 36 | Structural basis of TRPA1 inhibition by HC-030031 utilizing species-specific differences. Scientific Reports, 2016, 6, 37460. | 3.3 | 45 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Pressure Denaturation of Proteins and Peptides Studied by Molecular Dynamics Simulations. Seibutsu Butsuri, 2016, 56, 212-216. | 0.1 | 0 |
| 38 | 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. | 2.6 | 36 |
| 39 | Conformation study of É›-cyclodextrin: Replica exchange molecular dynamics simulations. Carbohydrate Polymers, 2016, 141, 99-105. | 10.2 | 15 |
| 40 | Comparison of Replica-Permutation Molecular Dynamics Simulations with and without Detailed Balance Condition. Journal of the Physical Society of Japan, 2015, 84, 074801. | 1.6 | 11 |
| 41 | Nonequilibrium and generalized-ensemble molecular dynamics simulations for amyloid fibril. AIP Conference Proceedings, 2015, , . | 0.4 | 0 |
| 42 | 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. | 3.3 | 12 |
| 43 | Molecular dynamics simulation study on the high-pressure behaviour of an AK16 peptide. Molecular Simulation, 2015, 41, 1035-1040. | 2.0 | 1 |
| 44 | Replica-permutation method to enhance sampling efficiency. Molecular Simulation, 2015, 41, 1021-1026. | 2.0 | 0 |
| 45 | 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. | 2.6 | 10 |
| 46 | Molecular dynamics of the structural changes of helical peptides induced by pressure. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2970-2981. | 2.6 | 14 |
| 47 | 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. | 3.3 | 34 |
| 48 | 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. | 1.6 | 3 |
| 49 | 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. | 2.6 | 44 |
| 50 | Amyloid Fibril Disruption by Ultrasonic Cavitation: Nonequilibrium Molecular Dynamics Simulations. Journal of the American Chemical Society, 2014, 136, 10549-10552. | 13.7 | 80 |
| 51 | High Pressure Effect on a Helical Peptide Studied by Simulated Tempering Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 611a. | 0.5 | 1 |
| 52 | Decomposition-order effects of time integrator on ensemble averages for the NosÃ©-Hoover thermostat. Journal of Chemical Physics, 2013, 139, 064103. | 3.0 | 8 |
| 53 | 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. | 3.3 | 58 |
| 54 | Onâ€theâ€fly reconstruction of freeâ€energy profiles using logarithmic meanâ€force dynamics. Journal of Computational Chemistry, 2013, 34, 1375-1384. | 3.3 | 8 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | 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. | 2.4 | 34 |
| 56 | Pressure-Induced Helical Structure of a Peptide Studied by Simulated Tempering Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2013, 4, 2079-2083. | 4.6 | 20 |
| 57 | Replica-Permutation Method with the Suwaâ€“Todo Algorithm beyond the Replica-Exchange Method. Journal of Chemical Theory and Computation, 2013, 9, 570-581. | 5.3 | 75 |
| 58 | 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. | 2.8 | 31 |
| 59 | Coulomb replicaâ€exchange method: Handling electrostatic attractive and repulsive forces for biomolecules. Journal of Computational Chemistry, 2013, 34, 622-639. | 3.3 | 27 |
| 60 | Cutoff Effect in the NosÃ©â€“PoincarÃ© and NosÃ©â€“Hoover Thermostats. Journal of the Physical Society of Japan, 2013, 82, 034001. | 1.6 | 2 |
| 61 | Free-energy calculation via mean-force dynamics using a logarithmic energy landscape. Physical Review E, 2012, 85, 066702. | 2.1 | 41 |
| 62 | Protein Simulations by Multibaricâ€“Multithermal Molecular Dynamics Algorithm. Journal of the Physical Society of Japan, 2012, 81, SA001. | 1.6 | 3 |
| 63 | 3E1058 Studies on a AÎ² fragment by the Coulomb replica-exchange method(Proteins:Structure,Oral) Tj ETQq1 1 0.784314 rgBT /Ove | 0.1 | 0 |
| 64 | Probing a Non-biaxial Behavior of Infinitely Thin Hard Platelets. Journal of the Physical Society of Japan, 2012, 81, 114003. | 1.6 | 0 |
| 65 | 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. | 2.6 | 82 |
| 66 | Generalized-Ensemble Algorithms for Simulations of Complex Molecular Systems. , 2012, , 69-101. | | 6 |
| 67 | Optimization of partial multicanonical molecular dynamics simulations applied to an alaninedipeptide in explicit water solvent. Physical Chemistry Chemical Physics, 2011, 13, 114-126. | 2.8 | 26 |
| 68 | Length Dependence of Polyglycine Conformations in Vacuum. Journal of the Physical Society of Japan, 2011, 80, 094801. | 1.6 | 5 |
| 69 | Conformational populations of ligandâ€sized molecules by replica exchange molecular dynamics and temperature reweighting. Journal of Computational Chemistry, 2010, 31, 1357-1367. | 3.3 | 17 |
| 70 | 3P071 multibaric-multithermal molecular dynamics simulations of a polyalanine(Protein: Property,The) Tj ETQq0 0 0 rgBT /Overlock 10 T | 0.1 | 0 |
| 71 | 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. | 1.5 | 4 |
| 72 | Replica-exchange method in van der Waals radius space: Overcoming steric restrictions for biomolecules. Journal of Chemical Physics, 2010, 132, 134105. | 3.0 | 46 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Examination of Temperature Dependence of Chemical Sputtering on Graphite by Comparing the Langevin and Berendsen Thermostats. Plasma and Fusion Research, 2010, 5, S2020-S2020. | 0.7 | 3 |
| 74 | 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 |
| 75 | Temperature and Pressure Dependence of Alanine Dipeptide Studied by Multibaricâ^'Multithermal Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 12038-12049. | 2.6 | 55 |
| 76 | Partial multicanonical algorithm for molecular dynamics and Monte Carlo simulations. Journal of Chemical Physics, 2008, 129, 124116. | 3.0 | 44 |
| 77 | 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. | 3.0 | 88 |
| 78 | Multibaricâ€“multithermal molecular dynamics simulation: generalized NosÃ©â€“PoincarÃ©â€“Andersen method. Molecular Simulation, 2007, 33, 91-96. | 2.0 | 0 |
| 79 | Multibaricâ€“Multithermal Molecular Dynamics Simulation of Alanine Dipeptide in Explicit Water. Bulletin of the Chemical Society of Japan, 2007, 80, 1114-1123. | 3.2 | 37 |
| 80 | Generalized-ensemble algorithms for molecular dynamics simulations. Molecular Simulation, 2007, 33, 47-56. | 2.0 | 33 |
| 81 | Equation of state and structural properties of the Weeks-Chandler-Andersen fluid. Journal of Chemical Physics, 2006, 124, 164507. | 3.0 | 56 |
| 82 | 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 |
| 83 | First derivative of the hard-sphere radial distribution function at contact. Journal of Physics Condensed Matter, 2006, 18, 7553-7558. | 1.8 | 8 |
| 84 | Multibaric-multithermal ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2006, 27, 379-395. | 3.3 | 53 |
| 85 | Hydrodynamics in a nanoscale liquid: comparisons with molecular dynamics in non-stationary processes. Molecular Physics, 2006, 104, 3751-3756. | 1.7 | 2 |
| 86 | Some physical properties of the Weeksâ€“Chandlerâ€“Andersen fluid. Molecular Simulation, 2006, 32, 45-50. | 2.0 | 24 |
| 87 | Stationary temperature profiles in a liquid nanochannel: Comparisons between molecular-dynamics simulation and classical hydrostatics. Physical Review E, 2006, 74, 061201. | 2.1 | 2 |
| 88 | Multibaricâ€“multithermal ensemble simulations for fluid systems. Physica A: Statistical Mechanics and Its Applications, 2005, 350, 150-158. | 2.6 | 0 |
| 89 | Molecular simulations in the multibaric-multithermal ensembles. Computer Physics Communications, 2005, 169, 317-321. | 7.5 | 1 |
| 90 | Comparisons between molecular dynamics and hydrodynamics treatment of nonstationary thermal processes in a liquid. Physical Review E, 2004, 70, 061206. | 2.1 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Monte Carlo simulations in generalized isobaric-isothermal ensembles. Physical Review E, 2004, 70, 026702. | 2.1 | 54 |
| 92 | Multibaricâ€“Multithermal Ensemble Simulation for Simple Liquids. Molecular Simulation, 2004, 30, 847-852. | 2.0 | 0 |
| 93 | Monte Carlo simulations in multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 383, 391-396. | 2.6 | 57 |
| 94 | Molecular dynamics simulations in the multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 391, 248-253. | 2.6 | 54 |
| 95 | Liquidâ€“Gas Phase Transitions Studied by Multibaricâ€“Multithermal Monte Carlo Simulations. Journal of the Physical Society of Japan, 2004, 73, 3304-3311. | 1.6 | 28 |
| 96 | New expression of the bulk viscosity. Physica A: Statistical Mechanics and Its Applications, 2003, 321, 207-219. | 2.6 | 29 |
| 97 | Nonequilibrium molecular dynamics simulations of a bubble. Physical Review E, 2003, 67, 045301. | 2.1 | 56 |
| 98 | Bulk viscosity in the case of the interatomic potential depending on density. Physical Review E, 2003, 67, 021205. | 2.1 | 7 |
| 99 | Simulational analysis of the local structure in liquid germanium under pressure. Physical Review B, 2002, 66, . | 3.2 | 28 |
| 100 | New formula for the bulk viscosity constructed from the interatomic potential and the pair distribution function. Journal of Chemical Physics, 2002, 116, 7400-7410. | 3.0 | 32 |
| 101 | Simulational study of liquid germanium under pressure. Journal of Non-Crystalline Solids, 2002, 312-314, 95-98. | 3.1 | 8 |
| 102 | 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. | 3.1 | 4 |
| 103 | Bulk viscosity in a density-dependent-potential system. Journal of Non-Crystalline Solids, 2002, 312-314, 260-264. | 3.1 | 2 |
| 104 | Approximate Formula for Bulk Viscosity. Journal of the Physical Society of Japan, 2002, 71, 685-688. | 1.6 | 13 |
| 105 | Method for liquidâ€“vapor coexistence curves by test-particle insertions in the canonical ensemble. Journal of Non-Crystalline Solids, 2001, 293-295, 715-718. | 3.1 | 3 |
| 106 | Expansion Type of Model Fluids. Journal of the Physical Society of Japan, 2001, 70, 1006-1009. | 1.6 | 14 |
| 107 | Molecular dynamics study of liquidâ€“vapor coexistence curves and supercritical fluids. Physica B: Condensed Matter, 2001, 296, 180-183. | 2.7 | 17 |
| 108 | Reliable Determination of the Liquid-Vapor Critical Point by theNVTPlus Test Particle Method. Journal of the Physical Society of Japan, 2001, 70, 1990-1994. | 1.6 | 49 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | The aspartate chemoreceptor Tar is effectively methylated by binding to the methyltransferase mainly through hydrophobic interaction. Molecular Microbiology, 2000, 36, 132-140. | 2.5 | 21 |
| 110 | The Relationship between the Metal-Nonmetal Transition and the Coordination Number in Divalent Systems. Progress of Theoretical Physics Supplement, 2000, 138, 255-256. | 0.1 | 0 |
| 111 | Liquid-Vapor Coexistence Curve and Fluid Structure. Progress of Theoretical Physics Supplement, 2000, 138, 253-254. | 0.1 | 4 |
| 112 | Liquidâ€“vapor coexistence curves of several interatomic model potentials. Journal of Chemical Physics, 2000, 113, 9162-9168. | 3.0 | 134 |
| 113 | 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. | 2.2 | 67 |