Atsushi Tokuhisa

List of Publications by Year
in descending order

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27 papers	1,700 citations	1040056 9 h-index	888059 17 g-index
28 all docs	28 docs citations	28 times ranked	2380 citing authors

#	Article	IF	Citations
1	A compact X-ray free-electron laser emitting in the sub-Ã¥ngstrÃ¶m region. Nature Photonics, 2012, 6, 540-544.	31.4	1,542
2	Classifying and assembling two-dimensional X-ray laser diffraction patterns of a single particle to reconstruct the three-dimensional diffraction intensity function: resolution limit due to the quantum noise. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 366-381.	0.3	24
3	High-Precision Atomic Charge Prediction for Protein Systems Using Fragment Molecular Orbital Calculation and Machine Learning. Journal of Chemical Information and Modeling, 2020, 60, 3361-3368.	5.4	22
4	Non-Gaussian behavior of elastic incoherent neutron scattering profiles of proteins studied by molecular dynamics simulation. Physical Review E, 2007, 75, 041912.	2.1	19
5	Hybrid approach for structural modeling of biological systems from X-ray free electron laser diffraction patterns. Journal of Structural Biology, 2016, 194, 325-336.	2.8	18
6	Single-particle XFEL 3D reconstruction of ribosome-size particles based on Fourier slice matching: requirements to reach subnanometer resolution. Journal of Synchrotron Radiation, 2018, 25, 1010-1021.	2.4	16
7	Hydration-coupled protein boson peak measured by incoherent neutron scattering. Physica B: Condensed Matter, 2006, 385-386, 871-873.	2.7	12
8	Enhanced Conformational Sampling with an Adaptive Coarse-Grained Elastic Network Model Using Short-Time All-Atom Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 2062-2074.	5.3	11
9	Proteinâ€“ligand binding affinity prediction of cyclinâ€dependent kinaseâ€2 inhibitors by dynamically averaged fragment molecular orbitalâ€based interaction energy. Journal of Computational Chemistry, 2022, 43, 1362-1371.	3.3	10
10	High-speed classification of coherent X-ray diffractionÂpatterns on the K computer for high-resolution single biomolecule imaging. Journal of Synchrotron Radiation, 2013, 20, 899-904.	2.4	6
11	Dynamical heterogeneity of protein dynamics studied by elastic incoherent neutron scattering and molecular simulations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 442, 356-360.	5.6	5
12	Exploring Successful Parameter Region for Coarse-Grained Simulation of Biomolecules by Bayesian Optimization and Active Learning. Biomolecules, 2020, 10, 482.	4.0	5
13	Characterization of X-ray diffraction intensity function from a biological molecule for single particle imaging. Biophysics and Physicobiology, 2019, 16, 430-443.	1.0	3
14	Coarse-Grained Diffraction Template Matching Model to Retrieve Multiconformational Models for Biomolecule Structures from Noisy Diffraction Patterns. Journal of Chemical Information and Modeling, 2020, 60, 2803-2818.	5.4	3
15	Calculation of Molecular-Structure-Based Damage Caused by Short-Pulse High-Intensity X-ray Lasers. Journal of the Physical Society of Japan, 2013, 82, 114301.	1.6	2
16	Intensity of Diffracted X-rays from Biomolecules with Radiation Damage Caused by Strong X-ray Pulses. Journal of the Physical Society of Japan, 2014, 83, 094301.	1.6	1
17	Single-Image Super-Resolution Improvement of X-ray Single-Particle Diffraction Images Using a Convolutional Neural Network. Journal of Chemical Information and Modeling, 2022, 62, 3352-3364.	5.4	1
18	1P066 Development of a computational method for single-molecule X-ray structure determination(Proteins-methodology,Poster Presentations). Seibutsu Butsuri, 2007, 47, S40.	0.1	0

#	Article	IF	Citations
19	3P-065 Theoretical approach for solving 3D structures of biomolecules with single-molecule X-ray diffraction patterns(The 46th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2008, 48, S137.	0.1	0
20	3P-069 Theory of single molecule imaging by X-ray free-electron laser(Protein:Measurement &) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0.1	0
21	2P011 Estimation of attainable structural resolution by computer simulation for single biomolecule imaging with X-ray Free Electron Laser(The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S83-S84.	0.1	0
22	3I1036 Estimation of attainable structural resolution by 3D imaging of biomolecules using X-ray free electron lasers(3I Protein: Measurement & Analysis 1,The 49th Annual Meeting of the Biophysical) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.1	0
23	3I1048 Phase retrieval from noisy x-ray diffraction patterns of single molecules(3I Protein:) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5 Butsuri, 2011, 51, S137.	0.1	0
24	3PS026 Automatic similarity identification of 2D diffraction patterns with noisy background for 3D coherent x-ray diffractive imaging(The 50th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2012, 52, S150.	0.1	0
25	2P077 Methodology of a single biomolecular structure determination for low-resolution data set obtained by X-ray Free Electron Laser(01E. Protein: Measurement & Analysis,Poster). Seibutsu Butsuri, 2013, 53, S171.	0.1	0
26	3P084 Examination of ab initio structural modeling for the pattern matching method using X-ray free electron laser(01E. Protein: Measurement & Analysis,Poster,The 52nd Annual Meeting of the) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 457	0.1	0
27	Decoupling Architecture for All-to-all Computation. , 2014, , .		0