

# Atsushi Tokuhisa

## List of Publications by Year in descending order

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Version: 2024-02-01

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	Enhanced Conformational Sampling with an Adaptive Coarse-Grained Elastic Network Model Using Short-Time All-Atom Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2062-2074.	5.3	11
2	Protein-ligand binding affinity prediction of cyclin-dependent kinase inhibitors by dynamically averaged fragment molecular orbital-based interaction energy. <i>Journal of Computational Chemistry</i> , 2022, 43, 1362-1371.	3.3	10
3	Single-Image Super-Resolution Improvement of X-ray Single-Particle Diffraction Images Using a Convolutional Neural Network. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3352-3364.	5.4	1
4	Coarse-Grained Diffraction Template Matching Model to Retrieve Multiconformational Models for Biomolecule Structures from Noisy Diffraction Patterns. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2803-2818.	5.4	3
5	High-Precision Atomic Charge Prediction for Protein Systems Using Fragment Molecular Orbital Calculation and Machine Learning. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3361-3368.	5.4	22
6	Exploring Successful Parameter Region for Coarse-Grained Simulation of Biomolecules by Bayesian Optimization and Active Learning. <i>Biomolecules</i> , 2020, 10, 482.	4.0	5
7	Characterization of X-ray diffraction intensity function from a biological molecule for single particle imaging. <i>Biophysics and Physicobiology</i> , 2019, 16, 430-443.	1.0	3
8	Single-particle XFEL 3D reconstruction of ribosome-size particles based on Fourier slice matching: requirements to reach subnanometer resolution. <i>Journal of Synchrotron Radiation</i> , 2018, 25, 1010-1021.	2.4	16
9	Hybrid approach for structural modeling of biological systems from X-ray free electron laser diffraction patterns. <i>Journal of Structural Biology</i> , 2016, 194, 325-336.	2.8	18
10	Intensity of Diffracted X-rays from Biomolecules with Radiation Damage Caused by Strong X-ray Pulses. <i>Journal of the Physical Society of Japan</i> , 2014, 83, 094301.	1.6	1
11	3P084 Examination of ab initio structural modeling for the pattern matching method using X-ray free electron laser (O1E. Protein: Measurement & Analysis, Poster, The 52nd Annual Meeting of the Tj ETQq1 1 0.784314rgBT /Overlock 10		
12	Decoupling Architecture for All-to-all Computation. , 2014, , .		0
13	High-speed classification of coherent X-ray diffraction patterns on the K computer for high-resolution single biomolecule imaging. <i>Journal of Synchrotron Radiation</i> , 2013, 20, 899-904.	2.4	6
14	Calculation of Molecular-Structure-Based Damage Caused by Short-Pulse High-Intensity X-ray Lasers. <i>Journal of the Physical Society of Japan</i> , 2013, 82, 114301.	1.6	2
15	2P077 Methodology of a single biomolecular structure determination for low-resolution data set obtained by X-ray Free Electron Laser (O1E. Protein: Measurement & Analysis, Poster). <i>Seibutsu Butsuri</i> , 2013, 53, S171.	0.1	0
16	A compact X-ray free-electron laser emitting in the sub-Ångström region. <i>Nature Photonics</i> , 2012, 6, 540-544.	31.4	1,542
17	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). <i>Seibutsu Butsuri</i> , 2012, 52, S150.	0.1	0
18	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. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2012, 68, 366-381.	0.3	24

#	ARTICLE	IF	CITATIONS
19	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 ETQq1 1 0.7843140gBT /Over		
20	3I1048 Phase retrieval from noisy x-ray diffraction patterns of single molecules(3I Protein:) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 Td Butsuri, 2011, 51, S137.	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	3P-069 Theory of single molecule imaging by X-ray free-electron laser(Protein:Measurement &) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	0
23	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
24	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
25	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
26	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
27	Hydration-coupled protein boson peak measured by incoherent neutron scattering. Physica B: Condensed Matter, 2006, 385-386, 871-873.	2.7	12