Koji Tsuda

List of Publications by Year
in descending order

94 papers	3,900 citations	117453 34 h-index	133063 59 g-index
98 all docs	98 docs citations	98 times ranked	3974 citing authors

#	Article	IF	Citations
1	Prediction of Low-Thermal-Conductivity Compounds with First-Principles Anharmonic Lattice-Dynamics Calculations and Bayesian Optimization. Physical Review Letters, 2015, 115, 205901.	2.9	343
2	Machine learning with systematic density-functional theory calculations: Application to melting temperatures of single- and binary-component solids. Physical Review B, 2014, 89, .	1.1	243
3	COMBO: An efficient Bayesian optimization library for materials science. Materials Discovery, 2016, 4, 18-21.	3.3	217
4	ChemTS: an efficient python library for de novo molecular generation. Science and Technology of Advanced Materials, 2017, 18, 972-976.	2.8	161
5	Designing Nanostructures for Phonon Transport via Bayesian Optimization. Physical Review X, 2017, 7, .	2.8	127
6	Ultranarrow-Band Wavelength-Selective Thermal Emission with Aperiodic Multilayered Metamaterials Designed by Bayesian Optimization. ACS Central Science, 2019, 5, 319-326.	5.3	121
7	Machine-learning prediction of the d-band center for metals and bimetals. RSC Advances, 2016, 6, 52587-52595.	1.7	113
8	Machine-Learning-Guided Mutagenesis for Directed Evolution of Fluorescent Proteins. ACS Synthetic Biology, 2018, 7, 2014-2022.	1.9	110
9	gBoost: a mathematical programming approach to graph classification and regression. Machine Learning, 2009, 75, 69-89.	3.4	106
10	Distribution Loss Minimization With Guaranteed Error Bound. IEEE Transactions on Smart Grid, 2014, 5, 102-111.	6.2	101
11	Crystal structure prediction accelerated by Bayesian optimization. Physical Review Materials, 2018, 2, .	0.9	94
12	Hunting for Organic Molecules with Artificial Intelligence: Molecules Optimized for Desired Excitation Energies. ACS Central Science, 2018, 4, 1126-1133.	5.3	91
13	Sparse modeling of EELS and EDX spectral imaging data by nonnegative matrix factorization. Ultramicroscopy, 2016, 170, 43-59.	0.8	90
14	Statistical significance of combinatorial regulations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 12996-13001.	3.3	82
15	Machine learning reveals orbital interaction in materials. Science and Technology of Advanced Materials, 2017, 18, 756-765.	2.8	78
16	EPIBLASTER-fast exhaustive two-locus epistasis detection strategy using graphical processing units. European Journal of Human Genetics, 2011, 19, 465-471.	1.4	74
17	Designing metamaterials with quantum annealing and factorization machines. Physical Review Research, 2020, 2, .	1.3	73
18	Machine-Learning-Assisted Development and Theoretical Consideration for the Al₂Fe₃Si₃ Thermoelectric Material. ACS Applied Materials & Interfaces, 2019, 11, 11545-11554.	4.0	69

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19	Acceleration of stable interface structure searching using a kriging approach. Japanese Journal of Applied Physics, 2016, 55, 045502.	0.8	65
20	Population-based De Novo Molecule Generation, Using Grammatical Evolution. Chemistry Letters, 2018, 47, 1431-1434.	0.7	63
21	PoSSuM: a database of similar protein-ligand binding and putative pockets. Nucleic Acids Research, 2012, 40, D541-D548.	6.5	62
22	Black-Box Optimization for Automated Discovery. Accounts of Chemical Research, 2021, 54, 1334-1346.	7.6	57
23	MDTS: automatic complex materials design using Monte Carlo tree search. Science and Technology of Advanced Materials, 2017, 18, 498-503.	2.8	52
24	Generating Ampicillin-Level Antimicrobial Peptides with Activity-Aware Generative Adversarial Networks. ACS Omega, 2020, 5, 22847-22851.	1.6	52
25	Structure prediction of boron-doped graphene by machine learning. Journal of Chemical Physics, 2018, 148, 241716.	1.2	46
26	Machine learning-driven optimization in powder manufacturing of Ni-Co based superalloy. Materials and Design, 2021, 198, 109290.	3.3	43
27	Data-driven approach for the prediction and interpretation of core-electron loss spectroscopy. Scientific Reports, 2018, 8, 13548.	1.6	42
28	Data-driven analysis of electron relaxation times in PbTe-type thermoelectric materials. Science and Technology of Advanced Materials, 2019, 20, 511-520.	2.8	42
29	Subspace classifier in the Hilbert space. Pattern Recognition Letters, 1999, 20, 513-519.	2.6	40
30	Integration of sonar and optical camera images using deep neural network for fish monitoring. Aquacultural Engineering, 2019, 86, 102000.	1.4	40
31	Application of Bayesian Optimization for Pharmaceutical Product Development. Journal of Pharmaceutical Innovation, 2020, 15, 333-343.	1.1	40
32	Optimization of a Heterogeneous Ternary Li₃PO₄â€“Li₃BO₃â€“Li₂SO₄ Mixture for Li-Ion Conductivity by Machine Learning. Journal of Physical Chemistry C, 2020, 124, 12865-12870.	1.5	40
33	An interpretable machine learning model for diagnosis of Alzheimer's disease. PeerJ, 2019, 7, e6543.	0.9	39
34	Functional Nanoparticles-Coated Nanomechanical Sensor Arrays for Machine Learning-Based Quantitative Odor Analysis. ACS Sensors, 2018, 3, 1592-1600.	4.0	38
35	Monte Carlo tree search for materials design and discovery. MRS Communications, 2019, 9, 532-536.	0.8	34
36	Mining Significant Substructure Pairs for Interpreting Polypharmacology in Drug-Target Network. PLoS ONE, 2011, 6, e16999.	1.1	34

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37	Bayesian optimization package: PHYSBO. Computer Physics Communications, 2022, 278, 108405.	3.0	33
38	Extracting straight lines by sequential fuzzy clustering. Pattern Recognition Letters, 1996, 17, 643-649.	2.6	32
39	Efficient error-tolerant query autocompletion. Proceedings of the VLDB Endowment, 2013, 6, 373-384.	2.1	31
40	Machine learning accelerates MD-based binding pose prediction between ligands and proteins. Bioinformatics, 2018, 34, 770-778.	1.8	31
41	Health Checkup and Telemedical Intervention Program for Preventive Medicine in Developing Countries: Verification Study. Journal of Medical Internet Research, 2015, 17, e2.	2.1	29
42	Efficient construction method for phase diagrams using uncertainty sampling. Physical Review Materials, 2019, 3, .	0.9	26
43	Asymptotic Properties of the Fisher Kernel. Neural Computation, 2004, 16, 115-137.	1.3	25
44	Transfer Learning to Accelerate Interface Structure Searches. Journal of the Physical Society of Japan, 2017, 86, 123601.	0.7	25
45	Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method. ACS Omega, 2019, 4, 13853-13862.	1.6	25
46	Machine-Learning-Guided Library Design Cycle for Directed Evolution of Enzymes: The Effects of Training Data Composition on Sequence Space Exploration. ACS Catalysis, 2021, 11, 14615-14624.	5.5	25
47	Protein functional class prediction with a combined graph. Expert Systems With Applications, 2009, 36, 3284-3292.	4.4	23
48	NMR-TS: de novo molecule identification from NMR spectra. Science and Technology of Advanced Materials, 2020, 21, 552-561.	2.8	23
49	Artificial Neural Networks Applied as Molecular Wave Function Solvers. Journal of Chemical Theory and Computation, 2020, 16, 3513-3529.	2.3	23
50	Realization of closed-loop optimization of epitaxial titanium nitride thin-film growth via machine learning. Materials Today Physics, 2021, 16, 100296.	2.9	22
51	Comparative Analysis of Patient-Matched PDOs Revealed a Reduction in OLFM4-Associated Clusters in Metastatic Lesions in Colorectal Cancer. Stem Cell Reports, 2021, 16, 954-967.	2.3	21
52	Fine-grained optimization method for crystal structure prediction. Npj Computational Materials, 2018, 4, .	3.5	20
53	Efficient recommendation tool of materials by an executable file based on machine learning. Japanese Journal of Applied Physics, 2019, 58, 098001.	0.8	20
54	Pushing property limits in materials discoveryviaboundless objective-free exploration. Chemical Science, 2020, 11, 5959-5968.	3.7	20

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55	CompRet: a comprehensive recommendation framework for chemical synthesis planning with algorithmic enumeration. Journal of Cheminformatics, 2020, 12, 52.	2.8	19
56	ROS-DET: robust detector of switching mechanisms in gene expression. Nucleic Acids Research, 2011, 39, e74-e74.	6.5	18
57	LAMPLINK: detection of statistically significant SNP combinations from GWAS data. Bioinformatics, 2016, 32, 3513-3515.	1.8	18
58	Using molecular dynamics simulations to prioritize and understand AI-generated cell penetrating peptides. Scientific Reports, 2021, 11, 10630.	1.6	17
59	Multi-way set enumeration in weight tensors. Machine Learning, 2011, 82, 123-155.	3.4	15
60	SketchSort: Fast All Pairs Similarity Search for Large Databases of Molecular Fingerprints. Molecular Informatics, 2011, 30, 801-807.	1.4	15
61	De novo creation of a naked eyeâ€“detectable fluorescent molecule based on quantum chemical computation and machine learning. Science Advances, 2022, 8, eabj3906.	4.7	14
62	Li-Ion Conductive Li3PO4-Li3BO3-Li2SO4 Mixture: Prevision through Density Functional Molecular Dynamics and Machine Learning. Bulletin of the Chemical Society of Japan, 2019, 92, 1100-1106.	2.0	13
63	Discovery of polymer electret material via de novo molecule generation and functional group enrichment analysis. Applied Physics Letters, 2021, 118, .	1.5	12
64	Machine Learning-Based Experimental Design in Materials Science. , 2018, , 65-74.		12
65	Determination of quasi-primary odors by endpoint detection. Scientific Reports, 2021, 11, 12070.	1.6	11
66	Continuous black-box optimization with an Ising machine and random subspace coding. Physical Review Research, 2022, 4, .	1.3	11
67	First-principles study of electronic structures and elasticity of Al2Fe3Si3. Journal of Physics Condensed Matter, 2021, 33, 195501.	0.7	10
68	Feâ€“Alâ€“Si Thermoelectric (FAST) Materials and Modules: Diffusion Couple and Machine-Learning-Assisted Materials Development. ACS Applied Materials & Interfaces, 2021, 13, 53346-53354.	4.0	10
69	Marginalized kernels for RNA sequence data analysis. Genome Informatics, 2002, 13, 112-22.	0.4	10
70	Improving the Accuracy of Proteinâ€Ligand Binding Mode Prediction Using a Molecular Dynamicsâ€Based Pocket Generation Approach. Journal of Computational Chemistry, 2018, 39, 2679-2689.	1.5	9
71	Molecular generation by Fast Assembly of (Deep)SMILES fragments. Journal of Cheminformatics, 2021, 13, 88.	2.8	9
72	RNA inverse folding using Monte Carlo tree search. BMC Bioinformatics, 2017, 18, 468.	1.2	8

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73	evERdock BAI: Machine-learning-guided selection of protein-protein complex structure. Journal of Chemical Physics, 2019, 151, 215104.	1.2	8
74	Efficient Search for Energetically Favorable Molecular Conformations against Metastable States via Gray-Box Optimization. Journal of Chemical Theory and Computation, 2021, 17, 5419-5427.	2.3	8
75	Matrix Factorization for Automatic Chemical Mapping from Electron Microscopic Spectral Imaging Datasets. Transactions of the Materials Research Society of Japan, 2016, 41, 333-336.	0.2	7
76	Minimizing the Cross Validation Error to Mix Kernel Matrices of Heterogeneous Biological Data. Neural Processing Letters, 2004, 19, 63-72.	2.0	6
77	Data integration for accelerated materials design via preference learning. New Journal of Physics, 2020, 22, 055001.	1.2	6
78	Leveraging algorithmic search in quantum chemical reaction path finding. Physical Chemistry Chemical Physics, 2022, 24, 10305-10310.	1.3	6
79	Sequential fuzzy cluster extraction and its robustness against noise. Systems and Computers in Japan, 1997, 28, 10-17.	0.2	5
80	Exploring Successful Parameter Region for Coarse-Grained Simulation of Biomolecules by Bayesian Optimization and Active Learning. Biomolecules, 2020, 10, 482.	1.8	5
81	CrySPY: a crystal structure prediction tool accelerated by machine learning. Science and Technology of Advanced Materials Methods, 2021, 1, 87-97.	0.4	5
82	Predictive Approaches for Low-Cost Preventive Medicine Program in Developing Countries. , 2015, , .		5
83	Generating reaction trees with cascaded variational autoencoders. Journal of Chemical Physics, 2022, 156, 044117.	1.2	5
84	Understanding the evolution of a de novo molecule generator via characteristic functional group monitoring. Science and Technology of Advanced Materials, 2022, 23, 352-360.	2.8	5
85	Efficient query autocompletion with edit distance-based error tolerance. VLDB Journal, 2020, 29, 919-943.	2.7	4
86	Bayesian Optimization in Materials Science. Lecture Notes in Physics, 2020, , 413-426.	0.3	4
87	DenseZDD: A Compact and Fast Index for Families of Sets. Algorithms, 2018, 11, 128.	1.2	3
88	Self-learning entropic population annealing for interpretable materials design. , 2022, 1, 295-302.		3
89	Multiple Testing Tool to Detect Combinatorial Effects in Biology. Methods in Molecular Biology, 2018, 1807, 83-94.	0.4	2
90	Integrating Incompatible Assay Data Sets with Deep Preference Learning. ACS Medicinal Chemistry Letters, 2022, 13, 70-75.	1.3	2

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91	Hybrid algorithm of Bayesian optimization and evolutionary algorithm in crystal structure prediction. Science and Technology of Advanced Materials Methods, 2022, 2, 67-74.	0.4	1
92	Can Machine Learning Guide Directed Evolution of Functional Proteins. Biophysical Journal, 2020, 118, 339a.	0.2	0
93	Machine-learning-guided Protein Design. Seibutsu Butsuri, 2021, 61, 177-179.	0.0	0
94	Ultra-Narrowband Wavelength-Selective Thermal Emitter Designed by Bayesian Optimization. The Proceedings of the Thermal Engineering Conference, 2018, 2018, 0135.	0.0	0