GÃ¡bor CsÃ¡nyi

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6310061/publications.pdf

Version: 2024-02-01

100	12,442	31902	38300
papers	citations	53 h-index	95 g-index

102	102	102	6716
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Implications of the BATTERY 2030+ AIâ€Assisted Toolkit on Future Lowâ€TRL Battery Discoveries and Chemistries. Advanced Energy Materials, 2022, 12, 2102698.	10.2	20
2	Atomic cluster expansion: Completeness, efficiency and stability. Journal of Computational Physics, 2022, 454, 110946.	1.9	47
3	Kernel charge equilibration: efficient and accurate prediction of molecular dipole moments with a machine-learning enhanced electron density model. Machine Learning: Science and Technology, 2022, 3, 015032.	2.4	15
4	Ranking the information content of distance measures. , 2022, 1, .		13
5	A Combined Machine Learning and High-Energy X-ray Diffraction Approach to Understanding Liquid and Amorphous Metal Oxides. Journal of the Physical Society of Japan, 2022, 91, .	0.7	7
6	Nested sampling for physical scientists. Nature Reviews Methods Primers, 2022, 2, .	11.8	40
7	A Hybrid Machine Learning Approach for Structure Stability Prediction in Molecular Co-crystal Screenings. Journal of Chemical Theory and Computation, 2022, 18, 4586-4593.	2.3	14
8	Gaussian approximation potential for amorphous SiÂ:ÂH. Physical Review Materials, 2022, 6, .	0.9	6
9	Origins of structural and electronic transitions in disordered silicon. Nature, 2021, 589, 59-64.	13.7	192
10	Data-efficient machine learning for molecular crystal structure prediction. Chemical Science, 2021, 12, 4536-4546.	3.7	41
11	Atomic permutationally invariant polynomials for fitting molecular force fields. Machine Learning: Science and Technology, 2021, 2, 025017.	2.4	22
12	Experimentally Driven Automated Machine-Learned Interatomic Potential for a Refractory Oxide. Physical Review Letters, 2021, 126, 156002.	2.9	28
13	Performant implementation of the atomic cluster expansion (PACE) and application to copper and silicon. Npj Computational Materials, 2021, 7, .	3.5	76
14	Machine learning potentials for extended systems: a perspective. European Physical Journal B, 2021, 94, 1.	0.6	81
15	Physics-Inspired Structural Representations for Molecules and Materials. Chemical Reviews, 2021, 121, 9759-9815.	23.0	247
16	Active Learning Training Strategy for Predicting O Adsorption Free Energy on Perovskite Catalysts using Inexpensive Catalyst Features. Chemistry Methods, 2021, 1, 444-450.	1.8	2
17	Machine learning force fields based on local parametrization of dispersion interactions: Application to the phase diagram of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>. Physical Review B, 2021, 104, .	1.1	29
18	Nested sampling for materials. European Physical Journal B, 2021, 94, 1.	0.6	13

#	Article	IF	Citations
19	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	23.0	384
20	Machine-learned interatomic potentials for alloys and alloy phase diagrams. Npj Computational Materials, 2021, 7, .	3.5	75
21	Predicting polarizabilities of silicon clusters using local chemical environments. Machine Learning: Science and Technology, 2021, 2, 045029.	2.4	1
22	Linear Atomic Cluster Expansion Force Fields for Organic Molecules: Beyond RMSE. Journal of Chemical Theory and Computation, 2021, 17, 7696-7711.	2.3	52
23	On the Role of Long-Range Electrostatics in Machine-Learned Interatomic Potentials for Complex Battery Materials. ACS Applied Energy Materials, 2021, 4, 12562-12569.	2.5	22
24	Machine learning interatomic potential developed for molecular simulations on thermal properties of Î²-Ga2O3. Journal of Chemical Physics, 2020, 153, 144501.	1.2	54
25	Incompleteness of Atomic Structure Representations. Physical Review Letters, 2020, 125, 166001.	2.9	103
26	Combining phonon accuracy with high transferability in Gaussian approximation potential models. Journal of Chemical Physics, 2020, 153, 044104.	1.2	29
27	An accurate and transferable machine learning potential for carbon. Journal of Chemical Physics, 2020, 153, 034702.	1.2	137
28	Machine-learned interatomic potentials by active learning: amorphous and liquid hafnium dioxide. Npj Computational Materials, 2020, 6, .	3.5	100
29	Mapping Materials and Molecules. Accounts of Chemical Research, 2020, 53, 1981-1991.	7.6	71
30	Machine learning driven simulated deposition of carbon films: From low-density to diamondlike amorphous carbon. Physical Review B, 2020, 102, .	1.1	44
31	A general-purpose machine-learning force field for bulk and nanostructured phosphorus. Nature Communications, 2020, 11, 5461.	5.8	72
32	Machine learning in chemical reaction space. Nature Communications, 2020, 11, 5505.	5.8	100
33	A machine learning based intramolecular potential for a flexible organic molecule. Faraday Discussions, 2020, 224, 247-264.	1.6	22
34	Learning the electronic density of states in condensed matter. Physical Review B, 2020, 102, .	1.1	57
35	Gaussian Process States: A Data-Driven Representation of Quantum Many-Body Physics. Physical Review X, 2020, 10, .	2.8	6
36	Hierarchical machine learning of potential energy surfaces. Journal of Chemical Physics, 2020, 152, 204110.	1.2	57

#	Article	IF	Citations
37	Functional movements of the GABA type A receptor. Physical Chemistry Chemical Physics, 2020, 22, 16023-16031.	1.3	4
38	Performance and Cost Assessment of Machine Learning Interatomic Potentials. Journal of Physical Chemistry A, 2020, 124, 731-745.	1.1	428
39	Partitioning of sulfur between solid and liquid iron under Earthâ€™s core conditions: Constraints from atomistic simulations with machine learning potentials. Geochimica Et Cosmochimica Acta, 2020, 291, 5-18.	1.6	23
40	Machine-Learning of Atomic-Scale Properties Based on Physical Principles. Lecture Notes in Physics, 2020, , 99-127.	0.3	4
41	Machine Learning of Atomic-Scale Properties Based on Physical Principles. , 2020, , 1911-1937.		3
42	Regularised atomic body-ordered permutation-invariant polynomials for the construction of interatomic potentials. Machine Learning: Science and Technology, 2020, 1, 015004.	2.4	46
43	First-principles study of alkali-metal intercalation in disordered carbon anode materials. Journal of Materials Chemistry A, 2019, 7, 19070-19080.	5.2	68
44	Machine Learning Interatomic Potentials as Emerging Tools for Materials Science. Advanced Materials, 2019, 31, e1902765.	11.1	389
45	De novo exploration and self-guided learning of potential-energy surfaces. Npj Computational Materials, 2019, 5, .	3.5	132
46	Machine-learned multi-system surrogate models for materials prediction. Npj Computational Materials, 2019, 5, .	3.5	96
47	Quantifying Chemical Structure and Machineâ€Learned Atomic Energies in Amorphous and Liquid Silicon. Angewandte Chemie - International Edition, 2019, 58, 7057-7061.	7.2	35
48	Quantifying Chemical Structure and Machineâ€Learned Atomic Energies in Amorphous and Liquid Silicon. Angewandte Chemie, 2019, 131, 7131-7135.	1.6	18
49	Equation of State of Fluid Methane from First Principles with Machine Learning Potentials. Journal of Chemical Theory and Computation, 2019, 15, 2574-2586.	2.3	40
50	Growth Mechanism and Origin of High <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:math> Content in Tetrahedral Amorphous Carbon. Physical Review Letters, 2018, 120, 166101.	2.9	128
51	Gaussian approximation potential modeling of lithium intercalation in carbon nanostructures. Journal of Chemical Physics, 2018, 148, 241714.	1.2	71
52	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. Journal of Chemical Physics, 2018, 148, 241725.	1.2	142
53	Data-Driven Learning of Total and Local Energies in Elemental Boron. Physical Review Letters, 2018, 120, 156001.	2.9	150
54	Data-driven learning and prediction of inorganic crystal structures. Faraday Discussions, 2018, 211, 45-59.	1.6	66

#	Article	IF	Citations
55	Development of a machine learning potential for graphene. Physical Review B, 2018, 97, .	1.1	142
56	Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems. Physical Review Letters, 2018, 120, 036002.	2.9	186
57	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. Molecular Simulation, 2018, 44, 866-880.	0.9	69
58	Screw dislocation structure and mobility in body centered cubic Fe predicted by a Gaussian Approximation Potential. Npj Computational Materials, 2018, 4, .	3.5	63
59	Machine Learning a General-Purpose Interatomic Potential for Silicon. Physical Review X, 2018, 8, .	2.8	222
60	Machine Learning of Atomic-Scale Properties Based on Physical Principles. , 2018, , 1-27.		6
61	Preconditioners for the geometry optimisation and saddle point search of molecular systems. Scientific Reports, 2018, 8, 13991.	1.6	8
62	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. Chemistry of Materials, 2018, 30, 7438-7445.	3.2	69
63	Reactivity of Amorphous Carbon Surfaces: Rationalizing the Role of Structural Motifs in Functionalization Using Machine Learning. Chemistry of Materials, 2018, 30, 7446-7455.	3.2	77
64	Modeling the Phase-Change Memory Material, Ge₂Sb₂Te₅, with a Machine-Learned Interatomic Potential. Journal of Physical Chemistry B, 2018, 122, 8998-9006.	1.2	102
65	Towards an atomistic understanding of disordered carbon electrode materials. Chemical Communications, 2018, 54, 5988-5991.	2.2	84
66	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 2879-2885.	2.1	170
67	Similarity Between Amorphous and CrystallineÂPhases: TheÂCaseÂofÂTiO₂. Journal of Physical Chemistry Letters, 2018, 9, 2985-2990.	2.1	78
68	Bayesian inference of the spatial distributions of material properties. Journal of the Mechanics and Physics of Solids, 2018, 118, 74-97.	2.3	26
69	Machine-learning based potential for iron: Plasticity and phase transition. AIP Conference Proceedings, 2018, , .	0.3	7
70	Nested Transition Path Sampling. Physical Review Letters, 2018, 120, 250601.	2.9	24
71	Achieving DFT accuracy with a machine-learning interatomic potential: Thermomechanics and defects in bcc ferromagnetic iron. Physical Review Materials, 2018, 2, .	0.9	175
72	Extracting Crystal Chemistry from Amorphous Carbon Structures. ChemPhysChem, 2017, 18, 873-877.	1.0	80

#	Article	IF	Citations
73	Machine learning based interatomic potential for amorphous carbon. Physical Review B, 2017, 95, .	1.1	431
74	Discovering the building blocks of atomic systems using machine learning: application to grain boundaries. Npj Computational Materials, 2017, 3, .	3.5	80
75	Machine learning unifies the modeling of materials and molecules. Science Advances, 2017, 3, e1701816.	4.7	488
76	Many-Body Coarse-Grained Interactions Using Gaussian Approximation Potentials. Journal of Physical Chemistry B, 2017, 121, 10934-10949.	1.2	93
77	Constant-pressure nested sampling with atomistic dynamics. Physical Review E, 2017, 96, 043311.	0.8	27
78	Polytypism in the ground state structure of the Lennard-Jonesium. Physical Chemistry Chemical Physics, 2017, 19, 19369-19376.	1.3	21
79	Structural simplicity as a restraint on the structure of amorphous silicon. Physical Review B, 2017, 95, .	1.1	18
80	A universal preconditioner for simulating condensed phase materials. Journal of Chemical Physics, 2016, 144, 164109.	1.2	46
81	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. Chemical Reviews, 2016, 116, 7501-7528.	23.0	314
82	Comparing molecules and solids across structural and alchemical space. Physical Chemistry Chemical Physics, 2016, 18, 13754-13769.	1.3	489
83	Exploration, Sampling, And Reconstruction of Free Energy Surfaces with Gaussian Process Regression. Journal of Chemical Theory and Computation, 2016, 12, 5100-5110.	2.3	72
84	Determining pressure-temperature phase diagrams of materials. Physical Review B, 2016, 93, .	1.1	49
85	Low Speed Crack Propagation via Kink Formation and Advance on the Silicon (110) Cleavage Plane. Physical Review Letters, 2015, 115, 135501.	2.9	25
86	<scp>G</scp>aussian approximation potentials: A brief tutorial introduction. International Journal of Quantum Chemistry, 2015, 115, 1051-1057.	1.0	442
87	Nested sampling for materials: The case of hard spheres. Physical Review E, 2014, 89, 022302.	0.8	31
88	Accuracy and transferability of Gaussian approximation potential models for tungsten. Physical Review B, 2014, 90, .	1.1	219
89	Free Energy Surface Reconstruction from Umbrella Samples Using Gaussian Process Regression. Journal of Chemical Theory and Computation, 2014, 10, 4079-4097.	2.3	48
90	Reactive Many-Body Expansion for a Protonated Water Cluster. Journal of Chemical Theory and Computation, 2014, 10, 68-75.	2.3	16

#	Article	IF	Citations
91	Machine-learning approach for one- and two-body corrections to density functional theory: Applications to molecular and condensed water. Physical Review B, 2013, 88, .	1.1	177
92	On representing chemical environments. Physical Review B, 2013, 87, .	1.1	1,440
93	Reply to â€œComment on 'Dynamic Catalyst Restructuring during Carbon Nanotube Growth'â€. ACS Nano, 2011, 5, 686-687.	7.3	0
94	Diffusive nested sampling. Statistics and Computing, 2011, 21, 649-656.	0.8	101
95	Efficient Sampling of Atomic Configurational Spaces. Journal of Physical Chemistry B, 2010, 114, 10502-10512.	1.2	89
96	Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons. Physical Review Letters, 2010, 104, 136403.	2.9	1,777
97	Gaussian Processes:â€‰ A Method for Automatic QSAR Modeling of ADME Properties. Journal of Chemical Information and Modeling, 2007, 47, 1847-1857.	2.5	188
98	Multiscale hybrid simulation methods for material systems. Journal of Physics Condensed Matter, 2005, 17, R691-R703.	0.7	36
99	Local invertibility and sensitivity of atomic structure-feature mappings. Open Research Europe, 0, 1, 126.	2.0	9
100	Free energies of Feâ€Oâ€Si ternary liquids at high temperatures and pressures: Implications for the evolution of the Earthâ€™s core composition. Geophysical Research Letters, 0, , .	1.5	2