Chenru Duan

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8422352/publications.pdf

Version: 2024-02-01

32 papers	1,253 citations	394390 19 h-index	414395 32 g-index
32 all docs	32 docs citations	32 times ranked	911 citing authors

#	Article	IF	Citations
1	A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chemical Science, 2019, 10, 7913-7922.	7.4	129
2	Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization. ACS Central Science, 2020, 6, 513-524.	11.3	114
3	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	47.7	110
4	Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. Industrial & Engineering Chemistry Research, 2018, 57, 13973-13986.	3.7	104
5	Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry. Inorganic Chemistry, 2019, 58, 10592-10606.	4.0	79
6	Zero-temperature localization in a sub-Ohmic spin-boson model investigated by an extended hierarchy equation of motion. Physical Review B, 2017, 95, .	3.2	73
7	Using Machine Learning and Data Mining to Leverage Community Knowledge for the Engineering of Stable Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 17535-17547.	13.7	71
8	Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metalâ€“Oxo Intermediate Formation. ACS Catalysis, 2019, 9, 8243-8255.	11.2	67
9	Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models. Journal of Chemical Theory and Computation, 2019, 15, 2331-2345.	5.3	66
10	Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. Journal of Physical Chemistry A, 2020, 124, 3286-3299.	2.5	48
11	Rapid Detection of Strong Correlation with Machine Learning for Transition-Metal Complex High-Throughput Screening. Journal of Physical Chemistry Letters, 2020, 11, 8067-8076.	4.6	40
12	Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design. Accounts of Chemical Research, 2021, 54, 532-545.	15.6	34
13	MOFSimplify, machine learning models with extracted stability data of three thousand metalâ€“organic frameworks. Scientific Data, 2022, 9, 74.	5.3	34
14	Data-Driven Approaches Can Overcome the Costâ€“Accuracy Trade-Off in Multireference Diagnostics. Journal of Chemical Theory and Computation, 2020, 16, 4373-4387.	5.3	28
15	Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery. Journal of Physical Chemistry Letters, 2021, 12, 4628-4637.	4.6	28
16	Semi-supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost. Journal of Physical Chemistry Letters, 2020, 11, 6640-6648.	4.6	27
17	Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles. Chemical Science, 2021, 12, 13021-13036.	7.4	23
18	New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts. Jacs Au, 2022, 2, 1200-1213.	7.9	23

#	Article	IF	Citations
19	Audacity of huge: overcoming challenges of data scarcity and data quality for machine learning in computational materials discovery. Current Opinion in Chemical Engineering, 2022, 36, 100778.	7.8	21
20	Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. Physical Chemistry Chemical Physics, 2020, 22, 19326-19341.	2.8	20
21	A Nonequilibrium Variational Polaron Theory to Study Quantum Heat Transport. Journal of Physical Chemistry C, 2019, 123, 17196-17204.	3.1	17
22	The study of an extended hierarchy equation of motion in the spin-boson model: The cutoff function of the sub-Ohmic spectral density. Journal of Chemical Physics, 2017, 147, 164112.	3.0	15
23	Dynamical scaling in the Ohmic spin-boson model studied by extended hierarchical equations of motion. Journal of Chemical Physics, 2019, 150, 084114.	3.0	14
24	Unusual Transport Properties with Noncommutative Systemâ€“Bath Coupling Operators. Journal of Physical Chemistry Letters, 2020, 11, 4080-4085.	4.6	13
25	Representations and strategies for transferable machine learning improve model performance in chemical discovery. Journal of Chemical Physics, 2022, 156, 074101.	3.0	11
26	Machine Learning for the Discovery, Design, and Engineering of Materials. Annual Review of Chemical and Biomolecular Engineering, 2022, 13, 405-429.	6.8	10
27	Detection of multi-reference character imbalances enables a transfer learning approach for virtual high throughput screening with coupled cluster accuracy at DFT cost. Chemical Science, 2022, 13, 4962-4971.	7.4	9
28	Machine Learning Models Predict Calculation Outcomes with the Transferability Necessary for Computational Catalysis. Journal of Chemical Theory and Computation, 2022, 18, 4282-4292.	5.3	9
29	Large-Scale Screening Reveals That Geometric Structure Matters More Than Electronic Structure in the Bioinspired Catalyst Design of Formate Dehydrogenase Mimics. ACS Catalysis, 2022, 12, 383-396.	11.2	5
30	Understanding the chemical bonding of ground and excited states of HfO and HfB with correlated wavefunction theory and density functional approximations. Journal of Chemical Physics, 2022, 156, 184113.	3.0	5
31	Exploiting Ligand Additivity for Transferable Machine Learning of Multireference Character across Known Transition Metal Complex Ligands. Journal of Chemical Theory and Computation, 2022, 18, 4836-4845.	5.3	4
32	Molecular orbital projectors in non-empirical jmDFT recover exact conditions in transition-metal chemistry. Journal of Chemical Physics, 2022, 156, 184112.	3.0	2